15–18 June 2026

RIGA | LATVIA

FUNCTIONAL MATERIALS & NANOTECHNOLOGIES

INTERNATIONAL CONFERENCE

BOOK OF ABSTRACTS 2026

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FM&NT 2026 - Abstract Book

WELCOME TO THE INTERNATIONAL CONFERENCE FUNCTIONAL MATERIALS AND NANOTECHNOLOGIES

FM&NT 2026 brings together scientists, students, companies, industry representatives, and experts from research institutes and universities across the Baltic Sea Region and beyond. The conference highlights the latest achievements in research, innovative solutions, and applications that foster international cooperation and advance the field of functional materials and nanotechnologies.

Representatives of **EIT RawMaterials** will join the event, offering insights into EU priorities, sector needs, and funding opportunities for commercialization and innovation. A dedicated session will introduce EIT RawMaterials innovation instruments, including the **KAVA Call**, designed to accelerate validated technologies toward market readiness.

The conference will include a **DEMO** exhibition of prototypes, technologies, and applied research, offering opportunities to connect with potential partners and explore new collaborations.

CONFERENCE TOPICS

Materials for Energy - batteries, supercapacitors, hydrogen, nuclear power.

Materials for Photonics - emission, detection, transformation of light, quantum photonics.

Ferroelectrics and Functional Materials - inorganic, organic, hybrid, low-dimensional, Van der Waals, topological ferroelectrics.

Microfluidics and Biomedical Technologies - organ-on-chip, lab-on-a-chip, biosensors, micro-nano robotics, biomaterials.

Theoretical Modelling of Functional Materials and Devices - prediction of next-generation materials, AI-based modelling.

Technologies and Devices - nanotechnologies, sensors, thin films, coatings, fibre optics, lasers.

Large-Scale Research Infrastructures, Science Policy and Collaboration - synchrotrons, neutron sources, FP10, international collaboration in materials research and innovation.

SCIENTIFIC COMMITTEE

- Andris Anspoks, Institute of Solid State Physics, University of Latvia
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- University of Latvia, Faculty of Science
- Smart Windows for Zero Energy Buildings (SWEB)

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CONFERENCE PROGRAM & SCHEDULE

June 15 – June 19

Time	Presentation Title & Speaker Details	Type / Duration
MONDAY, 15 JUNE		
11:00 – 13:00	Registration & coffee	
13:00 – 13:20	**Opening Ceremony**	
SESSION: Plenary *Chair: A. Sternbergs* Room: 110 (Alfa)		
13:20 – 13:50	Janis Timoshenko (DE) — Tracking Heterogeneous Structures of Electrocatalysts with Synchrotron- and Lab-based Operando XAS and Machine Learning	Plenary (40 min)
13:50 – 14:00	Christoph Deusen (DE) — 3D Optical Profilometer LEXT OLS5500	Plenary (20 min)
14:20 – 15:20	**Lunch**	
SESSION: 1-1 Ferroelectrics *Chair: J. Timoshenko* Room: 110 (Alfa)		
15:20 – 15:50	Andrei Kholkin (LV) — Magnetoelectric and ferroionic structures for microelectronic and biomedical applications	Invited (30 min)
15:50 – 16:20	Ernesto Alfaro-Moreno (PT) — Integrating Functional Material Design with Advanced Safety Assessment	Invited (30 min)
16:20 – 16:40	Svitlana Kopyl (PT) — Self-Assembled 2D Peptide Crystals and Thin Films	Oral (20 min)
16:40 – 17:00	S. Ramanavicius (LT) — Ferrite Based Functional Nanomaterials for Practical Applications	Oral (20 min)
SESSION: 1-2 Policy *Chair: A.Anspoks* Room: 103/104		
15:20 – 15:50	Ivars Ijabs (LV) — EU Research and Innovation Policy: the Main Challenges the Next Framework Programme (FP10)	Invited (30 min)
15:50 – 16:20	Alevtina Smekhova (DE) — X-ray absorption spectroscopy as an advanced characterization tool for compositionally complex systems	Invited (30 min)
16:20 – 16:40	Yaroslav Zhydachevskyy (PL) — Trap states engineering to improve persistent luminescence performance	Oral (20 min)
16:40 – 17:00	Sergii Ubizskii (UA) — The nanopowder synthesis and ceramics sintering of $Mg_{1-x}A_xAl_2O_4$ spinels	Oral (20 min)

SESSION: 1-3
Materials for Energy, ARMS Project Workshop
Room: 301

15:20–15:30	Hamed Pourkheirollah (FI) — A technical overview of the ARMS project	Oral (10 min)
15:30–15:45	Aleksandrs Volperts (LV) — Synthesis of biomass-based activated carbons for electrochemical applications	Oral (15 min)
15:45–16:05	Davis Kalnins (LV) — Supercapacitors: Principles and Electrochemical Measurement Techniques	Oral (20 min)
16:05–16:25	Remuel Vitto (FI) — ALD on supercapacitor electrodes and their electrochemical behavior	Oral (20 min)
16:25–16:50	Tero Pilvi (FI) — Towards high-volume scale-up of ALD coatings for battery and supercapacitor applications	Oral (25 min)
17:00 – 18:00	**Transfer to the Welcome Party at the ISSP UL**	
18:00 – 20:00	**Welcome Party at ISSP UL, 8 Kengaraga Street, Riga**	

TUESDAY, 16 JUNE		
08:30 – 09:00	Morning Registration	
SESSION: Plenary *Chair: A. Kholkin* Room: 110 (Alfa)		
09:00 – 09:40	Aymeric Robert (SE) — MAX 4U: the first fourth-generation lightsource upgrade	Plenary (40 min)
09:40 – 10:20	Lars Osterlund (SE) — Functional Chromogenic Nanostructures for Energy, Optics, and Display Technologies	Plenary (40 min)
10:20 – 10:40	**Coffee break**	
SESSION: 2-1 Energy *Chair: R. Merkle* Room: 110 (Alfa)		
10:40 – 11:10	Marit Kauk-Kuusik (EE) — Advancing Earth-Abundant Photovoltaic Materials	Invited (30 min)
11:10 – 11:40	Johannes Lischner (UK) — Hot electrons in plasmonic nanoparticles	Invited (30 min)
11:40 – 12:00	Ali Zavabeti (AU) — Liquid Metal Nano-Interface Engineering	Oral (20 min)
12:00 – 12:20	Evelina Dudutiene (LT) — Emission from bismuth quantum dots in annealed GaAsBi wells	Oral (20 min)
SESSION: 2-2 Modeling *Chair: R. Eglitis* Room: 103/104		
10:40 – 11:10	Eugene Kotomin (LV) — First principles computer modelling of advanced materials for fusion	Invited (30 min)
11:10 – 11:40	Denis Gryaznov (LV) — First-principles computational design of air electrode materials	Invited (30 min)
11:40 – 12:00	Ivan Novoseltsev — Investigation of crystal structures and optical properties of XH_3-$2xO_x$ oxyhydrides	Oral (20 min)
12:00 – 12:20	Ondrej Krejci (FI) — Accelerating Atomic Configuration Identification with Machine Learning	Oral (20 min)
SESSION: 2-3 Infrastructures *Chair: J. Purans* Room: 202		
10:40 – 11:10	Alexei Kuzmin (LV) — X-ray absorption spectroscopy study of polycrystalline $V_{1-x}Re_xO_2$ solid solution	Invited (30 min)
11:10 – 11:40	Aleksandr Kalinko (DE) — XAFS Spectroscopy at PETRA III: Capabilities and Applications	Invited (30 min)

11:40 – 12:00	Oksana Chukova — Optimization of Sol–Gel Synthesis Parameters for $LaAlO_3$ Nanoparticles	Oral (20 min)
12:00 – 12:20	Armi Tiihonen (SE) — Bayesian optimization machine learning method for high-throughput sample fabrication	Oral (20 min)
12:20 – 13:20	Lunch	
SESSION: Plenary *Chair: A. Kuzmin* Room: 110 (Alfa)		
13:20 – 14:00	Mikhail Brik (EE) — Crystal field theory, DFT and machine learning studies of phosphor materials	Plenary (40 min)
14:00 – 14:40	Tina Benda (SI) — EIT RawMaterials Infrastructure Presentation	Plenary (40 min)
14:40 – 15:00	**Coffee break**	
SESSION: 3-1 Energy *Chair: E. Kotomin* Room: 110 (Alfa)		
15:00 – 15:30	Rotraut Merkle (DE) — Protons in mixed-conducting perovskites: Why, how many, and how fast?	Invited (30 min)
15:30 – 16:00	Vytautas Klimavicius (LT) — NMR Investigation of NASICON-based materials	Oral (30 min)
16:00 – 16:20	Anna Pidluzhna (LV) — Technical Parameters and Principles of Charging in Li-Ion Batteries	Oral (20 min)
16:20 – 16:40	Alexey Rulev (CH) — Lattice Dynamic - Based Design of Light Ion Conductors	Oral (20 min)
16:40 – 17:00	Bejan Hamawandi (LV) — Versatile Solution-Based Synthesis of Thermoelectric Materials	Oral (20 min)
17:00 – 17:20	Pascal Henkel (FI) — How stable are mixed-metal chalcohalides?	Oral (20 min)
SESSION: 3-2 Devices *Chair: H. Klym* Room: 204		
15:00 – 15:30	Ruitao Wen (CN) — Electrochromic materials for visible and near infrared light modulation	Invited (30 min)
15:30 – 16:00	Smagul Karazhanov (LV) — Photochromic coatings: fundamentals and applications	Oral (30 min)
16:00 – 16:20	Arturs Bundulis (LV) — Polymer Photonics for Highly Nonlinear Host-Guest System Integration	Oral (20 min)
16:20 – 16:40	Jana Andzane (LV) — Hybrid Metal Oxide Nanowires for Bias-Free Photo-Driven Generation	Oral (20 min)

16:40 – 17:00	Arturs Mozers (LV) — Quantum Magnetometry in the University of Latvia	Oral (20 min)
17:00 – 17:20	Margarita Anna Zommere (LV) — Single Photone source and its development in Latvia	Oral (20 min)
SESSION: 3-3 Ferroelectrics *Chair: D. Gryaznov* Room: 201		
15:00 – 15:30	Volker Sittinger — Hybrid SALD–PVD approaches for electron contact layers	Invited (30 min)
15:30 – 16:00	Mantas Simenas (LT) — Emergence of a relaxor phase and dimensional tuning	Oral (30 min)
16:00 – 16:20	Yevhen Brych (IE) — Exploring ferroelectric and electrical properties in Cobalt Doped $BiFeO_3$	Oral (20 min)
16:20 – 16:40	Reinis Ignatans (LV) — Induced piezoelectric effect in cubic materials	Oral (20 min)
16:40 – 17:00	Roberts Eglitis (LV) — Ab initio calculations of ABO_3 Perovskite (001) Surfaces	Oral (20 min)
17:00 – 17:20	Liga Jasulaneca (LV) — Atomic Drums Without Order	Oral (20 min)
SESSION: Session D Seminar Room: 203		
15:00 – 16:30	EIT RawMaterials Informative seminar — Innovation Funding & Commercialisation	Seminar (90 min)
17:20 – 17:40	**Official Conference Photo**	
17:40 – 20:00	**Poster Session & Networking Reception**	

WEDNESDAY, 17 JUNE		
08:30 – 09:00	Morning Registration	
SESSION: Plenary *Chair: A. Sarakovskis* Room: 110 (Alfa)		
09:00 – 09:40	Marko Huttula (FIN) — Scaling research: From photoelectron-ion coincidences to hydrogen production	Plenary (40 min)
09:40 – 10:20	Miroslav Dramicanin (SRB) — Reimagining Luminescence Thermometry: Unleashing Spectral Analytics	Plenary (40 min)
10:20 – 10:40	**Coffee break**	
SESSION: 4-1 Photonics *Chair: A. Sarakovskis* Room: 110 (Alfa)		
10:40 – 11:10	Marco Kirm (EE) - Energy relaxation processes resulting in ultrafast cross-luminescence and intraband	Invited (30 min)
11:10 – 11:40	Dariusz Hreniak (PL) - Defect related luminescence properties of CaF_2 nanocrystals doped with rare-earth ions	Invited (30 min)
11:40 – 12:10	Halyna Klym (UA) - Positron annihilation approaches to the study of free-volume defects in functional nanostructured materials	Invited (30 min)
12:10 – 12:30	Viktorija Paramonova (LV) - Plasmonic Silver Nanoparticles: Synthesis and Optical Response	Oral (20 min)
SESSION: 4-2 Ferroelectrics *Chair: O. Chukova* Room: 202		
10:40 – 11:10	Edvardas Kazakevičius (LT) - In situ monitoring of crystallization in glassy mixed ionic-electronic conductors through impedance spectroscopy	Invited (30 min)
11:10 – 11:40	Marina Tyunina (FI) - Substrate-controlled point defects in thin films of perovskite oxides	Invited (30 min)
11:40 – 12:10	Juris Purans (LV) - Deposition of ZnO-Ga_2O_3 and Ir_2O_3-Ga_2O_3 thin films by reactive co-sputtering of liquid gallium	Invited (30 min)
12:10 – 12:30	Anna Marta Zeberga (LV) - Collagen–SPION Magnetic Nanocomposites for Small-Scale Oil Spill Remediation in Water Basins	Oral (20 min)
SESSION: 4-3 Devices *Chair: S. Karazhanov* Room: 725		
10:40 – 11:10	Kwang Leong Choy (CN) — Nanostructured Materials for a Sustainable Future	Invited (30 min)

11:10 – 11:40	Vittorio Morandi (IT) — EuroNanoLab distribuite nanofabrication facility for Europe	Invited (30 min)
11:40 – 12:10	Alexandr Dejneka (CZ) — From Optics to Integrated Innovation Ecosystems	Invited (30 min)
12:10 – 12:30	Anna Wojsiat Soosaar (EE) — Femtosecond Laser Treatment of Graphene for Gas Sensing Applications	Oral (20 min)
12:30 – 13:10	**Lunch**	
SESSION: 5-1 Photonics *Chair: R. Ignatans* Room: 110 (Alfa)		
13:10 – 13:30	Sergei Krylov (SK) — Study of thin Py films suitable for excitation of surface spin-wave	Oral (20 min)
13:30 – 13:50	Manivel Rajan (EE) — Luminescence properties of Cs_2HfF_6 using synchrotron radiation	Oral (20 min)
13:50 – 14:10	Boris Polyakov (LV) — Comparative Study of Thermal, Current-Induced, and Laser-Induced Melting	Oral (20 min)
SESSION: 5-2 Ferroelectrics *Chair: M. Tyunina* Room: 202		
13:10 – 13:40	Volker Eyert (FR) — Machine-Learned Potentials for Transition-Metal Oxides	Invited (30 min)
13:30 – 13:50	Donats Erts (LV) — Ionic thermoelectric energy harvesting using nanoconfined electrolytes	Oral (20 min)
13:50 – 14:10	Uday Pratap Singh Kushwah (EE) — First principles studies of ternary hexafluorides as scintillators	Oral (20 min)
SESSION: 5-3 Devices *Chair: M. Brik* Room: 725		
13:30 – 13:50	CHIN SHAN LUE (TW) — Single crystal growth of functional materials at NCKU	Oral (20 min)
13:10 – 13:40	Maksym Buryi (CZ) — Synthesis of advanced nanomaterials via plasma chemistry	Invited (30 min)
13:50 – 14:10	Ljubica Dacanin Far (RS) — Full-spectrum Principal Component Analysis-polynomial calibration	Oral (20 min)
14:10 – 14:30	Late-Breaking Short Project Presentations & Open Floor Discussions	Oral (20 min)
14:10 – 14:40	**Coffee break**	
14:40 – 18:00	**Excursion to the Jūrmala Open-Air Museum, Tīklu iela 1A, Jūrmala**	
18:30 – 22:00	**Conference Dinner at Semarah Hotel Lielupe, Jūrmala**	

THURSDAY, 18 JUNE		
08:30 – 09:00	Morning Registration	
SESSION: Plenary *Chair: A. Sternbergs* Room: 110 (Alfa)		
09:00 – 09:40	Juras Banys (LT) — Microwave Spectroscopy of Ferroelectrics and Related Materials	Plenary (40 min)
09:40 – 10:20	Viviana Andrea Claveria Pizarro (LV) — Microworlds on chips: microfluidics, biosensing	Plenary (40 min)
10:20 – 10:40	**Coffee break**	
SESSION: 6-1 Biomedical *Chair: M. Elksne* Room: 110 (Alfa)		
10:40 - 11:10	Damien Faivre (LV) — Controlling Swarms of Magnetic Micro- and Nanoswimmers	Invited (30 min)
11:10-11:40	Una Riekstina (LV) — Microfluidic PDAC-on-a-Chip for Patient-Specific Drug Testing	Oral (20 min)
11:40 - 12:10	Arunas Stirke (LT) — Advances in Microfluidic Electrochemical Biosensors for Biofilm Analysis	Oral (20 min)
12:10 - 12:30	Amit Blumberg (IL) - Turning Strategy into Practice: SWOT Analysis for Integring Microfluidic Rapid DNA Technologies	Oral (20 min)
SESSION: 6-2 Modeling *Chair: A. Popov* Room: 103/104		
10:40 - 11:10	Maytal Caspary Toroker (IL) — Charge transport through catalytic materials	Invited (30 min)
11:10-11:40	Vyacheslavs Kashcheyevs (LV) — Single-electron quantum technologies	Oral (20 min)
11:40 - 12:10	Ahmet Burak Baloglu (EE) — Enhanced thermal stability in graphene-based gas sensors	Oral (20 min)
SESSION: 6-3 Photonics Room: 205		
10:40 - 11:10	Paul Stradins (US) — Nanostructured Materials for Silicon Photovoltaics	Invited (30 min)
11:10-11:40	Viktorija Pankratova (FI) — Influence of europium ion doping on photoinduced properties	Oral (20 min)
11:40 - 12:10	Igors Mihailovs (LV) — Compute-Me-(Not): Bulky groups attached to nonlinear optical chromophores	Oral (20 min)

12:10 - 12:30	Arturs Medvids (LV) - Comparative Analysis of Nanostructures Formation in Semiconductors by Laser Irradiation and Stranski-Krastanov Methods	Oral (20 min)
Closing Ceremony & Awards Presentation Room: 110 (Alfa)		
12:30 – 12:45	**Closing Ceremony & Awards Presentation**	
12:45 – 13:15	**Closing Refreshments & Networking**	
Summer school ISSP, UL		
14:00 - 18:30	SWEB Summer school kickoff at ISSP, UL	
FRIDAY, 19 JUNE		
Summer school ISSP, UL		
9:30 - 17:40	SWEB Summer School on Functional Coatings and X-Chromic Materials	Educational

No.	TITLE	PARTICIPANT NAME	CONFERENCE SECTION
1	One-pot intrapore encapsulation of copper species in mesoporous SiO2 nanocomposites for durable antimicrobial surface coatings	**Aadil Shafi Bhat**	Ferroelectrics and Functional Materials
2	Na-SUBSTITUTED NdMnO3 PEROVSKITES: SYNTHESIS AND CHARACTERIZATION	**AIGUL DASTANKYZY**	Ferroelectrics and Functional Materials
3	Eco-Friendly Terpineol-Based Silver Nanoparticle Ink with Exceptional Stability and High Conductivity for Inkjet Printing	**Aleksandrs Novikovs**	Ferroelectrics and Functional Materials
4	Phase-Selective Synthesis of EuS2 and Eu3S4 via the Boron Chalcogen Mixture Method	**Aleksej Zarkov**	Ferroelectrics and Functional Materials
5	Enhanced Dark Redox Activity of CuO/CeO_2 Composites	**Ance Skalže**	Ferroelectrics and Functional Materials
6	Tannic Acid–Assisted Design of Ce-Modified CuO with Enhanced Redox Activity	**Anna Petrova**	Ferroelectrics and Functional Materials
7	Surface Functionalization-Driven Control of Magnetic Characteristics in $CoFe_2O_4$ Nanoparticles	**Aswathi Raveendran**	Ferroelectrics and Functional Materials
8	Dielectric Behavior and Triboelectric Output of TENGs Based on 0.80Na0.5Bi0.5TiO3-0.20BaTiO3/PDMS Composites	**Darya Meisak**	Ferroelectrics and Functional Materials
9	Molten salt synthesis towards preparation of Ruddlesden-Popper, perovskite and pyrochlore-type materials	**Dovydas Karoblis**	Ferroelectrics and Functional Materials
10	Hydrogen partial pressure as a key parameter in the reactive sputtering of photochromic YHO thin films	**Edvards Strods**	Ferroelectrics and Functional Materials
11	Formation mechanism of core–shell structures in lead-free ferroelectric ceramics via the diffusion method.	**Gusts Agafonovs**	Ferroelectrics and Functional Materials
12	Broad-band dielectric and Raman study of structural transformations in van der Waals ferrielectric CuInP2S6	**Juras Banys**	Ferroelectrics and Functional Materials
13	Impact and characteristics of oxygen vacancies in ferroelectric HfO2 based materials	**Katrīna Laganovska**	Ferroelectrics and Functional Materials
14	Electromechanically responsive materials based on electrospun polymer nanofibers	**Martynas Kinka**	Ferroelectrics and Functional Materials
15	High-Frequency Magnetic Characterization of CERN Fast Kicker Magnet Materials	**Sergejus Balciunas**	Ferroelectrics and Functional Materials
16	Synthesis, crystal structure and thermal behaviour of new high-entropy perovskite (Pr0.2Nd0.2Sm0.2Eu0.2Gd0.2)AlO3	**Sergii Ubizskii**	Ferroelectrics and Functional Materials
17	Photothermally Activated Shape-Memory Polymer–Silver Nanoparticle Composites for Light-Triggered 3D-Printed Actuators	**Virginija Vitola**	Ferroelectrics and Functional Materials
18	Preparation and characterisation of GaN-Al2O3-NbSe2 core-shell nanowires	**Luīze Dipāne**	Ferroelectrics and Functional Materials
19	Atomic Layer Deposition of ZnO Nanostructures onto Glass Wool	**Margarita Volkova**	Ferroelectrics and Functional Materials
20	PHOTO-ASSISTED ENERGY STORAGE IN AQUEOUS ZINC-ION BATTERIES USING BI2SE3–MWCNT CATHODES	**Gustavs Henrijs Zvaigzne**	Materials for Energy
21	ELECTROCHEMICAL PERFORMANCE OF CARBON NANOTUBES IN AQUEOUS ZINC ION BATTERIES	**Andrei Felsharuk**	Materials for Energy
22	ELECTROCHEMICAL PERFORMANCE OF CARBON NANOTUBES IN AQUEOUS ZINC ION BATTERIES	**Andrei Felsharuk**	Materials for Energy
23	Structure–Driven Electrochemical Behavior of NaOH-Activated Birch Carbons for Energy Storage	**Dāvis Kalniņš**	Materials for Energy
24	Discovery of photochromism with fast bleaching in oxygen-containing lanthanum hydride thin films	**Emija Letko**	Materials for Energy
25	Measurement of shallow dopants concentrations in polycrystalline silicon by low-temperature FTIR Spectroscopy	**George Chikvaidze**	Materials for Energy
26	The role of radiation-induced defect centres on spectroscopic properties of lithium orthosilicate, lithium metatitanate and their composites	**Guna Krieke**	Materials for Energy
27	Local Atomic Structure in Entropy-Engineered Thermoelectric Chalcogenides	**Inga Pudza**	Materials for Energy
28	Enhanced thermovoltage generation in multilayer AAO membranes via interface effects and tunable surface charge	**Irina Oliseveca**	Materials for Energy
29	Alder-based electrodes for supercapacitors	**Jūlija Hodakovska**	Materials for Energy
30	Characterisation of paramagnetic radiation-induced defect centres in biphasic Li4SiO4-Li2TiO3 ceramics under exposure to various types of ionising radiation	**Laura Dace Pakalniete**	Materials for Energy
31	Thermal properties for radiation-modified sheep wool fibers	**Liga Avotina**	Materials for Energy
32	Hydrogen Generation from Heterogeneous Aluminium Waste by Alkaline Hydrolysis	**Līga Grīnberga**	Materials for Energy
33	A comparative study of YAP:Bi and YAP:Mn phosphors: X-ray-, photo-luminescence and OSL response to irradiation	**Marina Koņuhova**	Materials for Energy

34	Influence of Chamber Wall Thickness on the Thermal Performance of a Liquid Piston Hydrogen Compressor	**Marina Koņuhova**	Materials for Energy
35	FLEXIBLE CNT-CHALCOGENIDE HYBRID STRUCTURES FOR SCALABLE THERMOELECTRIC ENERGY HARVESTING	**Parveen Sehrawat**	Materials for Energy
36	Thermoelectric Properties of Silver-Doped Copper Iodide / PEDOT:PSS Composites	**Renate Celmodejeva**	Materials for Energy
37	Ab initio calculations of the high voltage 5 Volt rechargeable Li ion battery cathode Li2CoMn3O8 and new battery anodes	**Roberts Eglitis**	Materials for Energy
38	Functional carbon aerogels as electrode materials for sodium-Ion energy harvesting and storage devices	**Rouz Barjoud**	Materials for Energy
39	The influence of the high energy (12,5 MeV) electron irradiation on optical materials with Mg-spinel structure	**Sergii Ubizskii**	Materials for Energy
40	Transparent WO_3/TiO_2 Nanocomposite Coatings with Enhanced Photochromic Switching for Smart Window Applications	**Tamara Tsebriienko**	Materials for Energy
41	Solvothermal Synthesis of Bismuth Selenide and Single-Walled Carbon Nanotube Heterostructures for Improved Charge Storage in Aqueous Zinc-Ion Batteries	**Viktorija Galaktionova**	Materials for Energy
42	Sb2Te3-Based Organic-Inorganic Thermoelectric Composites	**Adriana Mauručaite**	Materials for Energy
43	Paper production using green algae	**Jānis Poots**	Materials for Energy
44	Short-range structural distortions in (MgCoNiCuZn)O high-entropy oxide revealed by EXAFS spectroscopy	**Julija Lukaševiča**	Materials for Energy
45	X-ray absorption spectroscopy studies of protonation-induced electronic and structural changes in WO_3 nanoparticles	**Vitalijs Dimitrijevs**	Materials for Energy
46	Characterization of neutron induced defects in Al_2O_3 ceramics using optical absorption, TSL, and Raman methods	**Edgars Elsts**	Materials for Energy
47	Grains and crystallite size study of the optically transparent spinel ceramics	**Halyna Klym**	Materials for Energy
48	Visible Photoluminescence in Piezoelectric Diphenylalanine Thin Films	**Suvankar Mondal**	Materials for Energy
49	Characterization of Free Volume Transformations in MgAl2O4 Ceramics	**Halyna Klym**	Materials for Energy
50	Simulation of conductive networks in nanotube-based composites	**Halyna Klym**	Materials for Energy
51	Advanced flexible thermoelectric generator based on carbon nanotubes – inorganic semiconductor heterostructures	**Davis Gavars**	Materials for Energy
52	Integrated micro-hydrolysis system of sodium borohydride for powering flexible electronic devices	**Marinoiu Adriana**	Materials for Energy
53	Micro-Reactor Architecture with Capillary Separation and Multidirectional Phase Management	**Marinoiu Adriana**	Materials for Energy
54	Probing the Local Structure and Lattice Dynamics of Rhenium-Substituted VO_2 with Universal Machine Learning Potentials	**Pjotrs Žguns**	Materials for Energy
55	Comprehensive analysis regarding the development of flexible and ultra-light PEM fuel cells through the integration of advanced nanomaterials for wearable electronics	**Marinoiu Adriana**	Materials for Energy
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71	Optical absorption of interstitial oxygen in silicon dioxide.	**Linards Skuja**	Materials for Photonics
72	Laser processing as an alternative route for obtaining electroluminescent ZnS:Cu	**Madara Kļave**	Materials for Photonics
73	Excitonic and defect-related luminescence in $BaMgF_4$ ceramics under VUV excitation	**Marina Koņuhova**	Materials for Photonics
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77	Microwave-assisted synthesis of doped zinc sulfide electroluminescent phosphors	**Milena Dile**	Materials for Photonics
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79	Tuning the Luminescence Properties of Hackmanite with Zinc	**Pinja Tamminen**	Materials for Photonics
80	Comparative study of nano-ceramic and single crystalline dosimetric phosphor YAlO3:Bi	**Sergii Ubizskii**	Materials for Photonics
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85	LUMINESCENCE OF Tb/Eu3+-DOPED Y2.97-xNaxAl5O12 GARNETS UNDER SYNCHROTRON RADIATION	**Nataliya Krutyak**	Materials for Photonics
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88	Synthesis of Cu, Ag, and Au Nanoplates for In Situ SEM Studies of Thermal, Electrical, and Plasmonic Heating.	**Ligita Ostrovska**	Materials for Photonics
89	Ce3+-activated materials for optical temperature sensors in 0 °C – 400 °C range	**Linda Pujāte**	Materials for Photonics
90	Coupling between MoS2 and Plasmonic grating	**Chiao-Chih Lin**	Materials for Photonics
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92	Engineering Scalable Aptamer-Gold Interfaces for Rapid Malaria Diagnostics	**Edmunds Zutis**	Microfluidics and Biomedical technologies
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94	Specificity analysis of the GreenB1 aptamer in pancreatic ductal adenocarcinoma models: a comparative study of static and microfluidic environments	**Kristaps Sunteiks**	Microfluidics and Biomedical technologies
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104	Dual-window photoluminescence gas sensing with ultrathin Eu-doped ZnO films on black aluminium absorbers	**Jaroslav Otta**	Technologies and Devices
105	Electroluminescent Performance of OLEDs with Ag Nanoparticle-Modified PEDOT:PSS Layer	**Khrystyna Ivaniuk**	Technologies and Devices
106	Deposition optimization and characterization of structural and anticorrosion properties of HEA thin films obtained via DC Magnetron Sputtering	**Laura Madalina Cursaru**	Technologies and Devices
107	Carrier transport in CVD graphene field-effect transistors	**Linas Ardaravičius**	Technologies and Devices
108	Preperation and Photochromic Properties of Hybrid Co-doped TiO2/amino-PDMS Gels	**Loreta Abricka**	Technologies and Devices
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110	Crystal structure and mechanical properties of ALD-grown and thermally treated hafnium oxide–silicon oxide composite films	**Oliver Vanker**	Technologies and Devices
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113	Close-loop wavefront pre-compensated laser amplifier for structured light amplification	**Yuan-Yao Lin**	Technologies and Devices
114	Real-time Automated Identification and Quality Assessment of 2D Materials using Referring Expression Segmentation	**Wing-Sing Cheung**	Theoretical Modeling of Functional Materials and Devices
115	ML-Guided Screening of Heterojunction Photocatalysts for Green Hydrogen Production	**Abay Usseinov**	Theoretical Modeling of Functional Materials and Devices
116	Data-Driven Calibration of LED Illumination Angles in Fourier Ptychographic Microscopy	**Ajeem Samsudeen**	Theoretical Modeling of Functional Materials and Devices
117	EXAFS spectroscopy study of the temperature-dependent lattice dynamics of wurtzite ZnO	**Daria Zandberg**	Theoretical Modeling of Functional Materials and Devices
118	Advanced modeling methods to investigate oxygen defects in MgO	**Elina Kolesnikova**	Theoretical Modeling of Functional Materials and Devices
119	Bismuth modified SrTiO3 perovskites for green hydrogen production: DFT studies	**Guntars Zvejnieks**	Theoretical Modeling of Functional Materials and Devices
120	Computational study of the structural, electronic, vibrational and elastic properties of Na_2SiF_6 and Na_2SiF_6:Mn4+ phosphors	**Ilya Chevyakov**	Theoretical Modeling of Functional Materials and Devices
121	EPR and DFT investigation of neutron-radiation-induced defects in gallium gadolinium garnet	**Jekabs Cirulis**	Theoretical Modeling of Functional Materials and Devices
122	Modeling the Direct Current Sputtering Process for High-Entropy Alloys	**Laura Madalina Cursaru**	Theoretical Modeling of Functional Materials and Devices
123	Interpretation of EXAFS spectra of CeO2 using MACE, NequIP, and CHGNet Foundational Models	**Leons Stankevičs**	Theoretical Modeling of Functional Materials and Devices
124	MLIP Factory: An End-to-End, Ab-Initio-to-GPU Workflow for Radiation Damage in Complex Ionic Compounds	**Rostislavs Rostovskis**	Theoretical Modeling of Functional Materials and Devices
125	DFT-supported ML Design of Mn-Doped BiVO4 Photoanodes for Visible-Light-Driven Water Splitting	**Sergei Piskunov**	Theoretical Modeling of Functional Materials and Devices
126	The effective diffusion coefficient in inhomogeneous solids with inclusions. A comparison of 2D continous and discrete models	**Vladimir Kuzovkov**	Theoretical Modeling of Functional Materials and Devices
127	From DFT to ML for modeling of functional catalyst materials	**Vladislav Ivanistsev**	Theoretical Modeling of Functional Materials and Devices
128	Laser processing as an alternative route for obtaining electroluminescent ZnS:Cu	**Madara Kļave**	Materials for Photonics
129	Simultaneous in situ dielectric and crystallographic temperature dependent measurements	**Kaspars Jaundzems**	Ferroelectrics and Functional Materials

ABSTRACTS

of the PLENARY PRESENTATIONS

Alphabetically by Corresponding Authors

Microwave Spectroscopy of Ferroelectrics and Related Materials

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Saulius Rudys , Vilnius University
Sarunas Svirskas , Vilnius University
Vidmantas Kalendra , Vilnius University

The dielectric response of materials provides information about the orientational adjustment of dipoles and the translational adjustment of mobile charges present in a dielectric medium in response to an applied electric field. Microwave and terahertz dielectric spectroscopy of ferroelectrics and related materials enables the independent determination of the dielectric permittivity and loss in the dispersion region, as well as the parameters of the soft modes related to phase transitions. Besides scientific purposes, microwave dielectric measurements are of increasing importance in telecommunications related applications and the design of microwave circuit components. The magnetic properties are also of crucial importance. Dielectric and magnetic parameters fully characterize the manner in which electromagnetic waves propagate within the medium. The difficulties of making measurements on a wide range of materials over a wide frequency (and temperature) range have led to the development of various direct and indirect methods. Computers allow the computation of electromagnetic fields in entirely new measurement geometries and the use of numerical analysis in the direct measurement process. Each investigator employs the method adequate for the size and shape of a sample. The most important problem now is the rigorous mathematical solution of the microwave interaction with the samples in various geometries. Although there is now complete overlap and coverage of the radio frequency to the infrared band, the different experimental methods based on coaxial, waveguide, resonator and free – space technique is still divided and will be presented.

Keywords

Broad band dielectric spectroscopy, dielectric permittivity, magnetic susceptibility

EIT RawMaterials

Tina Benda , EIT RawMaterials

EIT RawMaterials is and Innovation Community supported by the European Institute of Innovation & Technology (EIT), is the world's largest consortium dedicated to strengthening Europe's raw materials sector. Its mission is to enable the sustainable competitiveness of the minerals, metals, and materials industries by driving innovation, education, and entrepreneurship across the full value chain, including exploration, mining, processing, recycling, and substitution.

EIT RawMaterials directly contributes to solving Europe's raw material supply challenges by advancing circular economy solutions, improving recycling technologies, and supporting material substitution. These efforts align closely with the EU's Critical Raw Materials Act and help reduce Europe's reliance on imported resources.

Opportunities for members include access to collaborative R&D, funding and investment instruments, start-up acceleration, entrepreneurial education, and extensive networking and matchmaking activities. Members also benefit from specialised training through the European Raw Materials Academy, supporting skill development across the sector.

Overall, EIT RawMaterials strengthens the mineral and materials sector by enhancing innovation capacity, improving resource security, supporting economic competitiveness, and preparing a skilled workforce for a resilient, circular, and sustainable European raw materials ecosystem.

Crystal field theory, DFT and machine learning studies of phosphor materials

Mikhail G. Brik , University of Tartu

Wide application of phosphor materials is based on emission properties of the transition metal (TM) and rare earth (RE) ions introduced as impurities (dopants) into crystalline solids. Complicated interplay of electronic and structural properties of host compounds with those of impurities determines the performance of such materials, areas and limitations of their use [1, 2].

In the present work an overview of applications of several different approaches (e.g. crystal field theory, DFT-based computational techniques [3-5], machine learning methods [6, 7]) to various inorganic crystalline materials doped with the TM and RE ions will be given and discussed, with special emphasis on how to identify location of the impurity ion's energy levels in the host band gap, calculate the splitting of the impurity ion's energy levels and predict their emission properties.

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Keywords

Optical Materials, Transition Metal and Rare Earth Ions, DFT, Crystal Field Theory, Machine Learning

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Microworlds on chips: microfluidics, biosensing, and scalable Lab-to-Fab technologies

Viviana Clavería , Institute of Solid State Physics, University of Latvia

Marianne Fenech , University of Ottawa, Canada

Microfluidics has reshaped biomedical technology by turning complex biology into controllable, measurable microsystems: organ-on-chip models to probe tissue function and drug response, lab-on-a-chip diagnostics that move assays from bench to bedside, and integrated biosensors that read chemistry and mechanics at micro and nano scales. By engineering flow, confinement, and biomaterial interfaces, microdevices create “microworlds” where physiology becomes reproducible and actionable [1-3].

In this talk, I will map this landscape of microtechnologies and show how shared design principles, shear and confinement control, robust biointerfaces, and embedded sensing, enable new functions and miniaturize phenomena that traditionally require millimeter- to macroscale setups. I will then use microcirculation as a case study where viscosity remains a technological challenge, highlighting why capturing microscale physics matters [4]. I will conclude with perspectives on how scalable microfluidic manufacturing can accelerate the transition from lab to fab, turning elegant prototypes into reproducible research tools and, ultimately, deployable biomedical technologies.

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Keywords

Microfluidics, Organ-on-chip, Lab-on-a-chip, Biosensing, Microcirculation

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3D Optical Profilometer LEXT OLS5500

Christoph Deusen , Evident

The Evident LEXT OLS5500 is a surface analyzing system using a combination of Confocal Laser Scanning Microscopy White Light Interferometry (Coherence Shift) and Focus Variation.

The system provides the advantage to inspect the same point on the sample surface with three analytical methods.

The combination of the three techniques provides the best optical resolution in x,y and z, big field of view and a high tolerance for big angles on the sample surface

Reimagining Luminescence Thermometry: Unleashing the Potential of Comprehensive Spectral Analytics for Unmatched Precision

Miroslav Dramicanin , University of Belgrade, Vinca Institute of Nuclear Sciences

The application of optically responsive materials in luminescence thermometry is crucial across various sectors, including materials engineering and medical diagnostics. This technique demands high accuracy and precision, traditionally achieved through two strategies: developing new luminescent materials with greater temperature sensitivity and refining analytical methods to interpret temperature data from luminescence signals. However, these approaches face limitations due to inherent photophysical properties and the narrow focus of current analysis methods, which often overlook much of the emission spectrum. As a result, challenges persist in optimizing the resolution and practical use of luminescence thermometry in dynamic settings.

This presentation introduces "Luminescence Thermometry 2.0," a novel approach that transcends existing limitations by utilizing the entire emission spectrum and sophisticated data analytics. Machine learning regression techniques, including principal component analysis and artificial neural networks, play a central role in this method. Case studies will illustrate how this comprehensive data-driven approach can significantly enhance the precision and accuracy of temperature measurements, even with existing experimental data. Moreover, this new direction simplifies practical implementation, offering more robust and accessible temperature sensing solutions in diverse real-world environments. Participants will gain insights into the deficiencies of traditional methodologies, the advantages of full-spectrum analysis, and the transformative potential of advanced data analytics in the field of luminescence thermometry.

Keywords

Luminescence, Luminescent thermometry, Machine learning, Principal component analysis

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Scaling research: From photoelectron-ion coincidences to photocatalytic solar hydrogen production

Marko Huttula , University of Oulu

Marko Huttula , Nano and Molecular Systems Research Unit, University of Oulu

Solar energy harvesting and the clean energy transition in general are thematic research topics receiving a lot of attention today. For example, the understanding of catalytic processes in the time domain and intermediate state level urges the development of fundamental research tools for imaging and characterisation towards chemically, temporally and spatially resolved in-situ and operando methods. In the present an overview on the physics lead hydrogen research at the University of Oulu and the lates advancements in photocatalytic hydrogen production aka solar hydrogen is provided including e.g. Zun-H spin-off. Focus is also given to methodology development in the field of catalysis and materials sciences. Examples are given on the use and development of synchrotron based and laboratory scale techniques (PEEM, APXPS, TAP) in the characterisation of novel nanoscale catalytic systems. Focus of the presentation is on analytical tools development in integration of advanced mass-spectroscopy and gas-phase electron spectroscopy with low-pressure steady-state and transient kinetic measurements. Examples are given on identification of isomeric-selective experiments and isomer discrimination of catalytic process during DME conversion.

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Keywords

photocatalytic hydrogen, solar energy, synchrotron,

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Functional Chromogenic Nanostructures for Energy, Optics, and Display Technologies

Lars Österlund , Umeå University

Chromogenic materials exhibit reversible changes in optical properties in response to external physical, chemical, or electrical stimuli, enabling dynamic control of light–matter interactions. In this talk, I will present recent advances in photochromic, thermochromic, and electrochromic oxyhydride and metal oxide materials, with a focus on nanostructuring and surface functionalization. I will discuss nanostructured anti-reflective coatings fabricated via colloidal lithography templating on iron-free glass, producing nanopillar architectures that exploit Mie scattering to achieve omnidirectional light management. Yttrium oxyhydride and superacid sulfated TiO_2 thin films were synthesized by magnetron sputtering, solid-state thermolysis and photo-fixation of SO_2 onto nano-templated surfaces, demonstrating reversible photochromism, ultraviolet blocking, and suppressed reflectance over wide incidence angles. Furthermore, bilayer TiO_2/VO_2 architectures reveal photothermally driven photocatalytic enhancement, while synergistic chemical and structural surface effects in YHO and sulfated TiO_2 coatings yield promising self-cleaning functionality. Finally, I will introduce a concept for “retina electronic paper” with human-eye resolution based on electrochromic WO_3 nanodisc metapixels with submicrometer dimensions, where an electrochemically induced insulator–metal transition enables tunable refractive index and absorption, achieving human-vision-limited resolution, high reflectance, and strong optical contrast. These results highlight the potential of chromogenic nanomaterials for smart coatings, solar control, and next-generation immersive display technologies.

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Keywords

Chromogenics, Chromogenic nanomaterials, Oxyhydride & metal oxide thin films, Nanostructured optical coatings, Photo-/thermo-/electrochromism, Smart coatings

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MAX 4U: the first fourth-generation lightsource upgrade.

Aymeric ROBERT , MAX IV Laboratory

Aymeric ROBERT , MAX IV Laboratory

MAX IV Laboratory is the Swedish national synchrotron radiation facility that comprises three accelerators with varying characteristics [1]. One of them, the 3 GeV storage ring, is the world's first fourth-generation synchrotron lightsource and pioneered the use of multibend achromat lattice approaches to provide access to ultrahigh brightness X-rays, thanks to its world-record small emittance of 328 pm·rad, as displayed in Fig. 1 (left). This has paved the way for new facility constructions and ambitious upgrade plans across the world.

While MAX IV has been operating since 2016, we are very excited about and actively discussing MAX 4^U [2], our plan to decrease the horizontal emittance from 328 pm·rad to below 75 pm·rad by the end of 2032, and remain at the forefront of possibilities in X-ray science. This is illustrated in Fig.1.(Right). This impressive milestone for a 3GeV medium energy storage ring should ensure the leadership, excellence, resilience, and relevance of Swedish research with X-rays for the next decades. We will discuss the current lattice design for MAX 4^U

Figure-Caption 1. Horizontal emittance (in units of picometer radian) of the European lightsources in 2016 (left) and early 2030s (Right) .

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Keywords

X-rays , Lightsouce , user facility , Research Infrastructure

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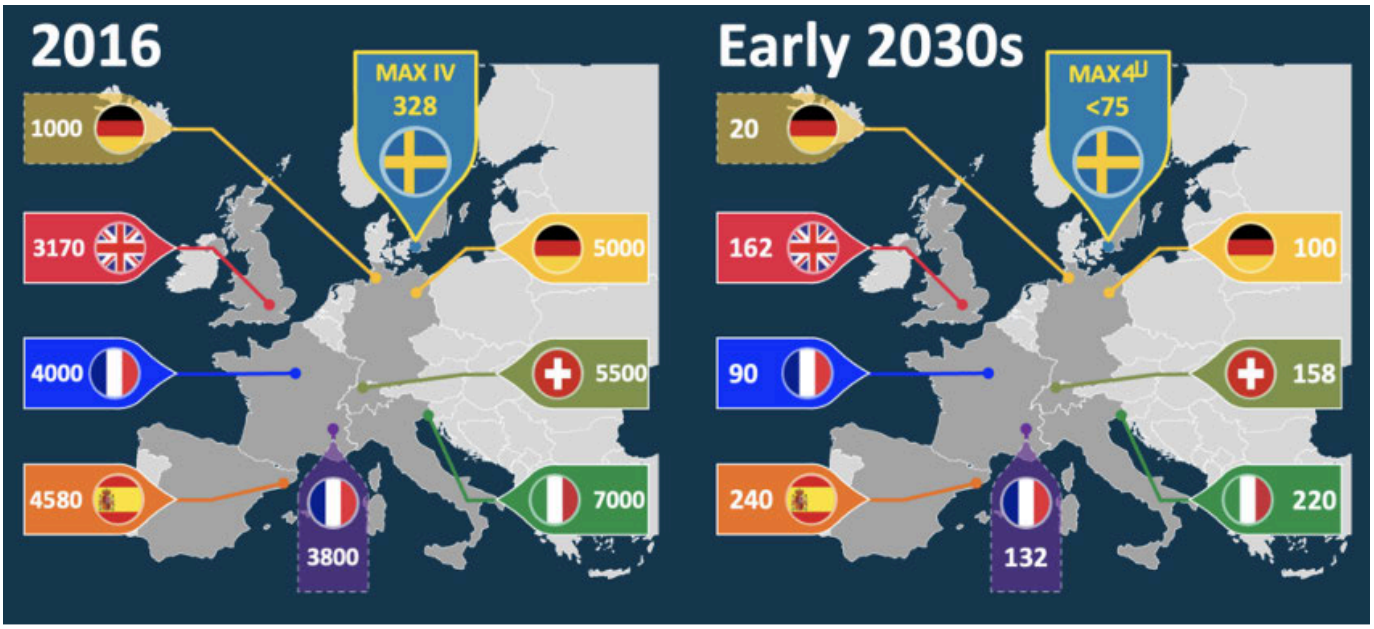
2016
MAX IV
328
1000
3170
4000
4580
5000
5500
7000
3800
Early 2030s
MAX4U
<75
20
162
90
240
100
158
220
132

Tracking Heterogeneous Structures of Electrocatalysts with Synchrotron- and Lab-based Operando XAS and Machine Learning

Janis Timoshenko , Fritz Haber Institut der Max Planck Gesellschaft

Identifying the structure-property relationships in functional materials and heterogeneous catalysts is a difficult task due to the dynamic transformation of active species on different time- and length-scales under working conditions. X-ray absorption spectroscopy (XAS) is a premier technique for addressing this issue due to its sensitivity to atomistic and electronic structure of the material and applicability to a broad range of different experimental conditions [1]. Nonetheless, the interpretation of XAS data remains challenging, especially if the investigated material is an evolving mixture of different species. Recent advances in operando XAS provide a solution to this problem. On one hand, lab-based XAS now allows one to screen large parameter spaces and design control experiments, and long-term studies that are incompatible with the traditional synchrotron beamtime access mode [2]. On the other hand, the developments in data science methods enable the interpretation of complex datasets containing contributions from multiple coexisting species. In particular, the development of machine learning methods for the interpretation of XAS spectra provides key insight for understanding the evolving structures of heterogeneous materials [3-6]. Here we demonstrate the potential of lab-based XAS and machine learning-based data analysis on an example of studies of working catalysts for CO2 electrocatalytic reduction [2,4] and oxygen evolution in alkaline electrolytes [6].

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Keywords

X-ray absorption spectroscopy, heterogeneous catalysis, operando studies, electrocatalysis, machine learning

ABSTRACTS

of the INVITED PRESENTATIONS

Alphabetically by Corresponding Authors

Integrating Functional Material Design with Advanced Safety Assessment

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The rapid development of functional engineered nanomaterials (ENMs) for applications in energy, electronics, coatings, and biomedicine requires parallel advances in predictive safety assessment. As control over size, morphology, and surface chemistry enables increasingly complex multifunctional materials, understanding nano–bio interactions becomes essential for safy and sustainability.

Conventional toxicity testing, relying on animal models and static 2D in vitro systems, often fails to capture the dynamic physicochemical processes governing nanomaterial behavior in biological environments. New Approach Methodologies (NAMs) provide an integrated, mechanism-based framework aligned with safe-and-sustainable-by-design principles.

Multicellular 2.5D/3D models, organoids, and organ-on-chip platforms enable realistic microenvironments and controlled exposure scenarios. Alternative in vivo models, including *Caenorhabditis elegans* and *Galleria mellonella*, allow efficient investigation of organism-level effects. In parallel, in silico tools such as quantitative structure–activity relationships and physiologically based kinetic modeling support predictive assessment based on material descriptors.

Together, these approaches create a synergistic toolbox connecting structure–property–function relationships with safety outcomes, accelerating the development of high-performance and safer nanotechnologies.

Keywords

Nanosafety, Nanotoxicology, Environmental Impact

Synthesis of the advanced nanomaterials by implementing principles of plasma chemistry

Maksym Buryi , Institute of Plasma Physics of the Czech Academy of Sciences

Advanced luminescent nanomaterials with improved optical performance and environmental stability were prepared using principles of plasma-chemical technologies. The studied systems included cesium lead bromide perovskite ($CsPbBr_3$, CPB), zinc oxide (ZnO) nanoparticles, and hybrid CPB/ZnO heterostructures. Plasma processing provides a highly reactive environment enabling controlled nucleation, crystallization, and surface modification of nanostructures.

$CsPbBr_3$ nanocrystals exhibiting strong green photoluminescence were synthesized and combined with ZnO nanoparticles to form heterostructures aimed at improving charge transfer and radiative recombination processes. ZnO nanoparticles were prepared both in undoped form and in erbium-doped variants (ZnO:Er), introducing additional luminescent centers and modifying emission pathways.

Organic pigments were used as a protective covering of the nanomaterial systems to enhance luminescent properties and partially shield the perovskite nanocrystals from moisture. The synthesized nanomaterials were also covered with polystyrene, improving stability and processability.

Optical characterization revealed enhanced emission intensity, higher light yield, and modified luminescence kinetics, indicating that plasma-chemical synthesis combined with hybrid material design is a promising route for efficient and stable luminescent nanomaterials.

Keywords

Plasma Chemical Technologies, $CsPbBr_3$ provskite nanocrystals, ZnO and ZnO:Er nanorods, $CsPbBr_3$/ZnO heterostructures, Luminescent nanocomposites

Acknowledgements

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Charge transport through catalytic materials

Maytal Caspary Toroker , Technion

Functional materials are important for applications in the fields of catalysis and renewable energy. Specific functionalities include charge transport through electronic material components as well as catalytic reactivity on material surfaces. In the talk, I will advocate that there is a relation between charge transport efficiency and reactivity, and therefore developing novel algorithms that calculate both are important for better understanding of intrinsic material limitations. We cover our latest results in developing and using charge transport calculation methods and demonstrate them on catalytic materials. Our home code is developed on a user-friendly GUI and enables to use widely available Density Functional Theory results as input. The methodology is demonstrated on several semiconducting materials.

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Keywords

charge transport simulations, computational materials modeling, density functional theory

Nanostructured Materials for a Sustainable Future: Eco-Friendly Design, Processing, and Performance

Kwang Leong Choy , Duke Kunshan University

This contribution explores how eco-friendly nanostructured materials serve as a cornerstone for solving critical global challenges in energy, environment, and functional applications, while actively enabling a sustainable future. The focus is on the rational design and development of such nanostructured functional materials—specifically tailored for clean energy generation and storage technologies, including photovoltaics, hydrogen production, and lithium-ion batteries. A key innovation lies in sustainable fabrication: we employ non-vacuum, scalable, and environmentally benign materials processing methods, including aerosol-assisted chemical vapour deposition (AACVD), to produce high-performance nanostructured materials and coatings. The deposition mechanism is elucidated at the molecular level, revealing how precise control over precursor chemistry, aerosol dynamics, and process parameters governs the nucleation, growth, and final architecture of the nanostructures. Critically, we demonstrate how these process controls directly influence material properties—and thereby determine device performance. Sustainability is embedded throughout, as the use of earth-abundant elements eliminates reliance on toxic or scarce resources, while the AACVD process operates under ambient pressure with low energy input. By systematically linking nanostructure engineering, green chemistry principles, and functional performance, this work provides a pathway toward advanced materials that are not only highly efficient but also inherently sustainable.

Keywords

Eco-friendly nanostructured materials, Sustainable fabrication, Aerosol-assisted chemical vapour deposition (AACVD), Clean energy storage and conversion

From Optics to Integrated Innovation Ecosystems: Interdisciplinarity as a Strategic Tool for European Competitiveness

Alexandr Dejneka , FZU - Institute of Physics of the Czech Academy of Sciences

Over the past decade, the Division of Optics at the Institute of Physics of the Czech Academy of Sciences has transformed from a discipline-oriented research unit into an interdisciplinary deep-tech ecosystem integrating optics, materials science, plasma technologies, laser engineering, biophysics, additive manufacturing, and digital innovation. A decisive turning point was the establishment of our first spin-off company CARDAM in 2016, which initiated long-term industrial cooperation and fundamentally reshaped our strategic thinking. Close interaction with industry revealed a critical requirement: companies need rapid and coordinated access to physics-based characterization, chemical synthesis, computational modelling, as well as biological and medical experimentation. To meet this need, we built strong internal interdisciplinary bridges, including advanced biointerface and biophotonics laboratories, enabling seamless collaboration between physical sciences and life sciences. This approach was institutionalized through the National Centre of Competence MATCA and expanded via the Brain4Industry Innovation Centre within the European Digital Innovation Hubs network, providing SMEs structured access to advanced technologies and digital solutions. A central pillar of this ecosystem is strategic talent management through the Radius Development Centre, which connects students, researchers, universities, and industry partners, supports international mobility and internships, and creates structured career pathways. Our experience demonstrates that interdisciplinarity combined with proactive talent cultivation is essential for delivering agile, market-relevant solutions and strengthening Europe's technological resilience and competitiveness.

Keywords

Interdisciplinary research, Technology transfer, International cooperation

Machine-Learned Potentials for Transition-Metal Oxides

Volker Eyert , Materials Design SARL

Volker Eyert , Materials Design

In the past two to three decades, Machine-Learned Potentials (MLPs) have established as an indispensable approach to advanced materials research, which allows to access increasingly larger systems at longer time scales and thereby to deepen our understanding of real materials [1]. This talk will illustrate the progress in the field with examples from the MedeA computational environment of Materials Design. The presentation ranges from a discussion of the basic concepts to challenges in creating efficient training sets and application of MLPs in practice.

A particular intriguing class of materials are the transition-metal oxides, which are of critical importance in many different fields such as energy production and storage (photovoltaics, batteries, fuel cells, hydrogen production), electronic devices (electrochromic, piezoelectric), and catalysis. Vanadium dioxide is one of the most prominent oxides of this class due to a temperature-induced phase transition at 340 K offering a large variety of applications, e.g., in smart windows, thermal coating, and memory devices. At the same time, the origin of the simultaneous occurrence of distinct structural distortions and the loss of metallic conductivity in the low-temperature phase is still a matter of dispute [2,3]. This talk reports on molecular-dynamics simulations in an NPT ensemble using an MLP generated from meta-GGA DFT calculations, which reproduced the structural changes occurring at the phase transition and the transition temperature in very good agreement with experimental data, allow to identify the relevant structural order parameters and thereby bring clarity to the decade-long controversial discussions about the phase transition.

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Keywords

Machine-Learned Potentials, Multiscale Simulations, Transition-Metal Oxides, Phase Transition

Ferroelectrics and Functional Materials, Microfluidics and Biomedical technologies

Microfluidics and Biomedical technologies

Controlling Swarms of Magnetic Micro- and Nanoswimmers

Damien Faivre , University of Latvia

The first magnetic microswimmer has now been described more than 20 years ago. Over the years, several actuation schemes have been described, and a continuous parallel has been encountered between biological objects as a source of inspiration, and synthetic counterparts. However, magnetism as a fueling source of motion has prevailed for synthetic devices, because of the non-invasive, untethered and precise control capability. However, if the three-dimensional control of single entities has effectively proven practical, controlling multiple devices in a swarm is still a challenging task. Here, I will present several approaches developed in my group to tackle this difficulty for a variety of microswimmers' type.

Keywords

magnetotactic bacteria, swarms, magnetic microswimmer

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Materials for Energy, Theoretical Modeling of Functional Materials and Devices

Theoretical Modeling of Functional Materials and Devices

First-principles computational design of air electrode materials

Denis Gryaznov , Institute of Solid State Physics, University of Latvia

Denis Gryaznov , Institute of Solid State Physics, University of Latvia
Andrew Chesnokov , Institute of Solid State Physics, University of Latvia
Yuri Mastrikov , Institute of Solid State Physics, University of Latvia
Guntars Zvejnieks , Institute of Solid State Physics, University of Latvia
Rotraut Merkle , Max Planck Institute for Solid State Research, Germany
Eugene Kotomin , Institute of Solid State Physics, University of Latvia

Triple-conducting perovskite oxides, possessing mobile oxide ion vacancies, protons, and electron holes, are used as air electrode materials for protonic ceramic electrochemical cells. Owing to this triple conduction property, they are challenging for both experimental and theoretical investigations and require deeper insight into the mechanisms governing defect concentrations and mobilities at atomistic level.

Density functional theory (DFT) calculations are a powerful tool for investigating defect behavior, as they enable a detailed analysis of atomic and electronic structure. We used $BaFeO_3$ as a model system 1) to uncover the mechanisms responsible for the complex triple conductivity 2) to assess its potential as a promising air electrode material 3) to develop and advance DFT simulations for material design by bridging fundamental understanding and electrode application oriented properties.

The dependences of the most relevant material properties on the Fe oxidation state were determined via high-throughput calculations of numerous defect configurations, and analyzed thoroughly [1]. These properties include proton migration energies [1-3], hydration energies [1-2] (see Figure), and oxygen vacancy formation energies [1, 4]. Chemical bonding characteristics, as well as chemical expansion effects, were examined with respect to electronic structure changes induced by the defect formation. The proton conductivity in $BaFeO_3$ was assessed for the first time using a machine learning force field method. We identified key descriptors that allow for reliable estimation and prediction of relevant materials properties for application as an air electrode. Our approach and interpretations can undoubtedly be extended to other triple-conducting perovskite oxides.

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Keywords

protonic ceramic electrochemical cells, BaFeO3, DFT+U, oxygen vacancies, protons, hydration energy, migration energy

Acknowledgements

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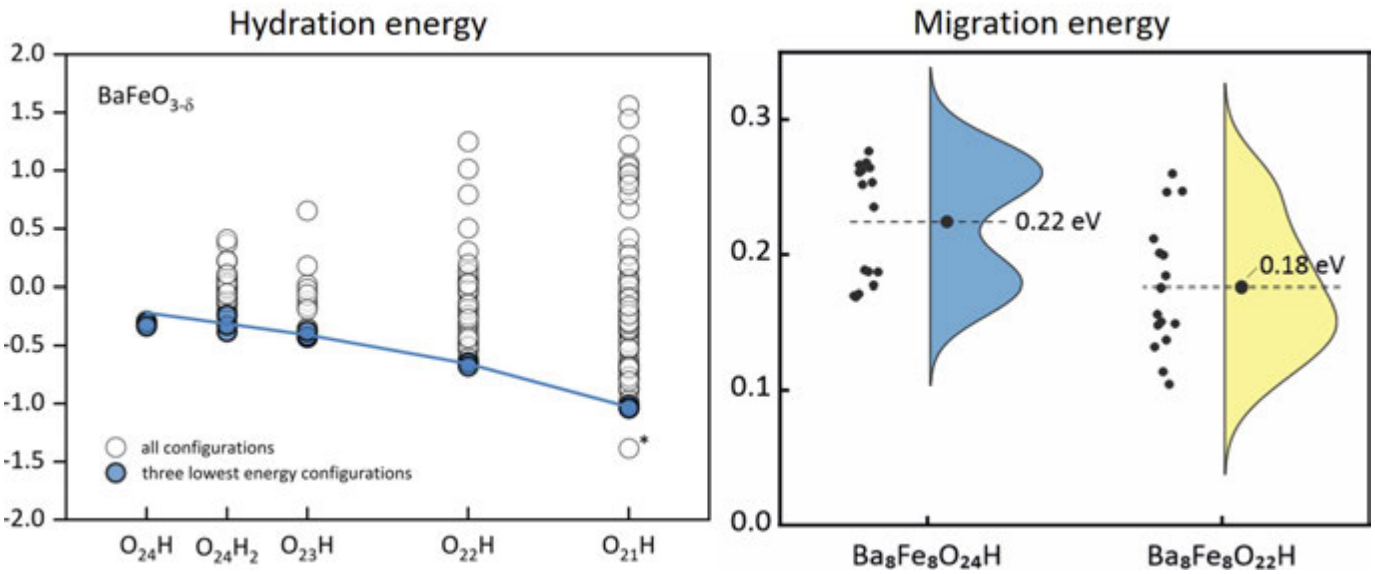

Defect related luminescence properties of CaF2 nanocrystals doped with rare-earth ions

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Andris Antuzevičs , Institute of Solid State Physics, University of Latvia
Anatolijs Šarakovskis , Institute of Solid State Physics, University of Latvia
Dariusz Hreniak , Institute of Low Temperature and Structure Research, Polish Academy of Sciences

A series of calcium fluoride (CaF_2) nanoparticles doped with various concentrations of rare-earth (RE) ions (Yb^{3+}, Er^{3+}, Tm^{3+}) was synthesised using the co-precipitation method. The X-ray diffraction measurements confirmed the cubic structure of the fluorite within all dopants concentration range, although slight lattice distortions were observed at higher doping levels. The transmission electron microscopy (TEM) images revealed well dispersed nanoparticles with an average size of 10 nm. High-resolution TEM images have enabled the direct visualisation of the distribution of impurity clusters located at Ca^{2+} sites within these nanocrystals, as well as their statistical analysis. Based on the vibrational spectroscopy (Attenuated Total Reflection Fourier Transform Infrared and Raman) structural distortions were confirmed to occur upon doping with RE ions. The emission spectra exhibited luminescence typical of the used RE ions. Additional measurements with deep UV (12 – 4 eV) were performed to analyse defect related emission in CaF_2 nanoparticles. Preliminary measurements of thermoluminescence curves and electron paramagnetic resonance spectra have been carried out to investigate the existence of defects that could be used as trapping centres in the persistent luminescence process.

Keywords

luminescence, rare-earth ions, defects

Acknowledgements

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Large-Scale Research Infrastructures, Science Policy and Collaboration

Large-Scale Research Infrastructures & Science Policy

EU Research and Innovation Policy: the Main Challenges the Next Framework Programme (FP10)

Ivars Ijabs , European Parliament

This presentation examines the evolving priorities and structural challenges facing European Union research and innovation policy in the context of the forthcoming Tenth Framework Programme (FP10). As the EU seeks to strengthen its global competitiveness, technological sovereignty, and resilience amid geopolitical instability, climate transition, and rapid digital transformation, FP10 is expected to play a central role in shaping Europe's innovation landscape beyond 2027.

The presentation analyses the main policy debates surrounding FP10, including the balance between excellence and cohesion, the simplification of funding instruments, the role of mission-oriented research, and the integration of industrial competitiveness with sustainability objectives. Particular attention is devoted to widening participation across Member States, improving synergies between EU and national funding schemes, and enhancing the commercialization of research outcomes. The discussion also addresses growing concerns regarding administrative burden, stakeholder inclusiveness, strategic autonomy, and Europe's capacity to compete with major global innovation actors such as the United States and China.

By exploring recent policy proposals, institutional discussions, and stakeholder perspectives, the presentation highlights both opportunities and tensions shaping the future of EU research governance. It argues that FP10 will need to reconcile scientific excellence with societal impact while ensuring flexibility, inclusiveness, and long-term strategic vision in an increasingly complex global environment.

Large-Scale Research Infrastructures, Science Policy and Collaboration

Large-Scale Research Infrastructures & Science Policy

XAFS Spectroscopy at PETRA III: Capabilities and Applications of the P64 and P65 beamlines

Aleksandr Kalinko , DESY

X-ray Absorption Fine Structure (XAFS) spectroscopy is a powerful tool for probing the local atomic and electronic structure of materials under realistic conditions. At the PETRA III storage ring, the P64 and P65 beamlines provide advanced capabilities for XAFS measurements across a broad range of scientific fields, including catalysis, energy materials, and functional materials.

Both beamlines support conventional transmission and fluorescence XAS, coupled with a wide variety of sample environments, including cryostat, gas-flow reactor for operando measurements, and user-provided custom cells.

The P64 beamline is optimized for high-flux XAFS spectroscopy, extending capabilities to sub-second quick-EXAFS measurements, high-resolution X-ray emission spectroscopy (XES), and high-energy-resolution fluorescence-detected XANES (HERFD-XANES). Additionally, we are currently establishing optical pump–X-ray probe XAS/XES for time-resolved studies and XANES tomography. These capabilities enable investigations of structural and electronic dynamics in dilute systems and operando environments.

In this presentation, we provide an overview of the instrumentation and experimental possibilities at the P64 and P65 beamlines. Selected scientific examples illustrate how XAFS methodologies can be applied to investigate oxidation-state changes, local coordination environments, and reaction dynamics in materials. Together, these beamlines provide a versatile platform for state-of-the-art XAFS spectroscopy.

Keywords

PETRA III, XAFS, XES, P64, P65

Photochromic coatings: fundamentals and applications

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Juris Purans , Institute of Solid State Physics, University of Latvia, Riga, Latvia

Yttrium oxyhydride ($YH_{3-2x}O_x$, YHO) is a mixed-anion material that exhibits properties not accessible in conventional single-anion systems. Synthesized through reactive magnetron sputtering to form $YH_2-\delta$ followed by controlled oxidation [1, 2] , YHO shows a distinctive photochromic response under ambient conditions. Upon exposure to sunlight or visible/UV illumination, it transitions from a highly transparent state (T > 85%) to a darkened state (T ≈ 20%) with nearly wavelength-independent absorption. These characteristics make YHO a strong candidate for smart windows, protective eyewear, helmet visors, and automotive glazing [3, 4], with roll-to-roll commercialization already initiated by industry partners such as Sunphade [5]. Today, the study of YHO and other rare-earth metal oxyhydrides is an increasingly attractive research field.

This talk will summarize recent progress on the physical and optical properties of YHO, including tunable transparency, switching kinetics, and stability under repeated cycling.
Temperature-dependent transition dynamics and long-term durability studies will be discussed, with emphasis on improving chemical robustness and accelerating response times for large-area applications. Advances in theoretical understanding such as predicted crystal structures of oxidized hydrides, hydrogen-related band structure modifications, and light-induced lattice breathing will also be highlighted. Additionally, the presentation will cover deposition strategies for small- and large-area substrates, prototype development, and functional testing in both laboratory and outdoor environments, including insights from roll-to-roll fabrication.

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Keywords

Chromogenic Materials, new materials, mixed anion materials, scalable methods of deposition, crystal structure prediction

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Single-electron quantum technologies

Vyacheslavs Kashcheyevs , University of Latvia

Universality of electrical charge quantization and the fundamental nature of the Planck constant are the foundational principles of electrical quantum metrology where macroscopic quantum phenomena (quantum Hall and Josephson effects) are routinely employed in commercial high-precision measurements systems. Recent advances in high-fidelity manipulation of discrete electrons in metrological current sources [1] open up a new resource for quantum technologies 2.0 [2] with individual electrons propagating in semiconductor circuits in direct analogy to photons. We discuss an electron quantum optics toolbox of circuit elements for on-demand emission, transformation, and read-out of single-electron wave-packets, emphasizing the unique advantages of beamsplitters [3,4,5] with the dispersion tuneable by the field effect and the non-linearity mediated by controlled Coulomb interaction. Envisioned applications are quantum-limited sensors for picosecond scale electrical signals and eventually an all-electronic quantum information platform interfaceable with other cryogenic on-chip technologies.

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Keywords

quantum technologies, single-electron devices, metrology, quantum optics

Advancing Earth-Abundant Photovoltaic Materials through Smart Processing Design

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Achmad Nasyori , Tallinn University of Technology

Photovoltaics (PV) are central to achieving global zero-emission energy goals, yet the market remains dominated by silicon technologies that depend on energy-intensive processing and increasingly constrained material supply chains. Earth-abundant kesterite Cu_2ZnSnS_4 (CZTS) is a promising alternative absorber composed of non-toxic and widely available elements. Owing to its suitable bandgap and strong light absorption, CZTS is attractive for thin-film, tandem, and indoor photovoltaic applications. However, the performance of pure-sulfide CZTS devices has historically been limited by structural disorder, defect-driven recombination, and interfacial losses.

In this work, we demonstrate that controlling the synthesis pathway and post-fabrication thermal treatment is crucial for improving device performance. First, we develop a solution-based fabrication route processed entirely under ambient air, showing that precursor design combined with post-annealing of the complete device significantly enhances junction quality and suppresses recombination, leading to substantial efficiency improvements.

Second, we show that engineering the sulfurization process improves absorber crystallinity and reduces bulk recombination. Importantly, we identify the cooling rate after device annealing as a previously underexplored but powerful parameter. Rapid cooling stabilizes favorable defect configurations, improves band alignment at the absorber/buffer interface, and enhances the back contact, resulting in reduced voltage losses and improved charge collection. Devices prepared using this approach reach efficiencies above 11% and exhibit excellent thermal stability during prolonged aging.

These findings highlight thermal pathway engineering as a simple, scalable strategy for advancing efficient and durable kesterite-based functional materials for photovoltaic applications.

Keywords

inorganic semiconductors, photovoltaics, thin films

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In situ monitoring of crystallization in glassy mixed ionic-electronic conductors through impedance spectroscopy

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Algimantas Kežionis , Vilnius University, Faculty of Physics
Tomas Šalkus , Vilnius University, Faculty of Physics
Maciej Nowagiel , Warsaw University of Technology, Faculty of Physics
Tomasz Płociński , Warsaw University of Technology, Faculty of Materials Science and Engineering
Tomasz K. Pietrzak , Warsaw University of Technology, Faculty of Physics

In situ, the temporal evolution of broadband impedance spectra of the glassy mixed ionic-electronic conductor Na3VTi(PO4)2F3 was examined by heat-treating the sample near its glass-transition temperature (T_g = 740 K). Several relaxation processes of charge carriers were identified in the spectra, and the distribution of relaxation times (DRT) method was employed for analysis. Initially, a single, moderately broad, bell-shaped DRT peak was observed, corresponding to the sole relaxation process in the glassy phase. Over time, this peak shifted towards longer relaxation times, broadened, and split into a double peak, with a third, broader peak emerging in the far region of lower relaxation times. After 7 hours, the double peak evolved into a relatively regular bell shape, representing the crystalline phase. The evolution of the DRT over 7 hours was illustrated by fitting the prominent DRT double peak to two distinct Gaussian bells. These Gaussian fits were used to determine the time-dependent phase composition of the mixed glassy-crystalline sample. The third peak was attributed to the relaxation process occurring in the inter-grain area.

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Keywords

Impedance Spectroscopy, Distribution of relaxation times, Crystallization

Acknowledgements

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Magnetoelectric and ferroionic structures for microelectronic and biomedical applications

Andrei Kholkin , Institute of Solid State Physics

Ferroelectric materials are widely used due to their reversible polarization, high dielectric constant, and remarkable piezoelectric and pyroelectric effects. The functionality of ferroelectrics can be extended by using a combination of these materials with ferromagnetics and ionic conductors at the nanoscale dimensions. In this presentation, ferroionic thin films combining ferroelectricity with ionic phenomena of fast charge recombination and electrodic functionalities will be first considered. The concept of tunable polarization in CeO_2 thin films induced by the built-in polarization of $BaTiO_3$ (BTO) thin-film interface, which is buried under the CeO_2 layer, will be introduced. We found that the ceria layer punctually replicates the polarization of BTO via a dynamic reconfiguration of its intrinsic defects, i.e., oxygen vacancies and small polarons. Tunable oxidative or reducing properties dictated by polarization also arise at such surfaces. This tunability opens up the perspectives of using ferroionics for wireless electrochemically enhanced catalysis. Another example of tunable nanostructures is magnetoelectric (ME) core-shell nanoparticles. These composites, prepared by soft hydrothermal synthesis, are characterized by excellent biocompatibility and show a large ME response mediated by the remote magnetic field. The intriguing physical properties of such structures will be considered, and their usefulness for various catalytic and biomedical applications will be shown.

Keywords

Ferroelectrics, ferroionics, magnetoelectrics, core-shell structures

Acknowledgements

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Energy relaxation processes resulting in ultrafast cross-luminescence and intraband luminescence in ternary fluorides

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Alexander Vanetsev , Institute of Physics, University of Tartu
Vitali Nagirnyi , Institute of Physics, University of Tartu

Scintillator materials have a wide range of application from simple ionizing radiation detection to sophisticated medical and scientific solutions, where superior time-resolution is required. Cross-luminescence (CL) and intraband luminescence (IBL) are ultrafast intrinsic emissions due to radiative recombination of electrons from the valence band with holes in the outermost core band [1] and electron or hole transitions within the conduction or valence band [2], respectively. Alongside Cherenkov radiation, these emissions have potential to achieve the much sought-after sub-nanosecond time resolution. Over recent years, we have been studying ternary hexafluorides possessing complex electronic band structure, responsible for a rich luminescence spectrum exhibiting both fast CL and IBL [3]. The energy gaps between the hybridized states of a split valence band promote the IBL transitions with decay times in tens and hundreds of ps. The wide bandgap of fluorides containing heavy elements is shown to be beneficial for observing both ultrafast CL and prompt Cherenkov radiation.

This contribution will present experimental results obtained, in particular, at the setup for time-resolved luminescence studies with excellent time resolution of ~30 ps, designed together with the FemtoMAX beamline team at the MAX IV Lab in Lund [4]. The basics of relaxation processes leading to ultrafast emissions and relevant experimental methods will be discussed (see Fig. 1).

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Keywords

Ultrafast emissions, cross-luminescence, intraband luminescence, ternary fluorides, scintillator, FemtoMAX beamline

Acknowledgements

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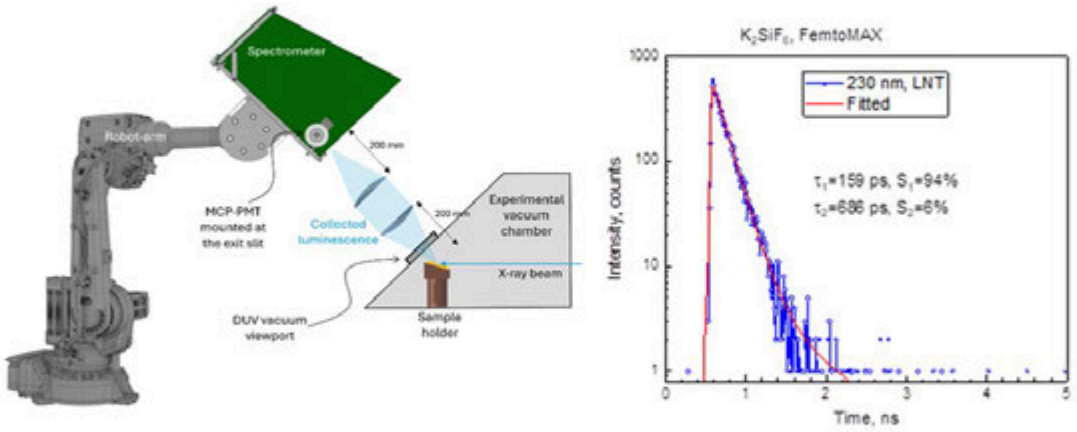

Figure 1. The operation scheme of the setup at the FemtoMAX beamline (left panel). A decay curve of an ultrafast luminescence at 230 nm recorded from a K_2SiF_6 sample at 80 K (right panel).

NMR Investigation of NASICON-based materials for Aqueous Batteries Applications

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Solid-state NMR is a powerful experimental technique that detects transitions between nuclear energy levels at strong magnetic fields. Combined with MAS and numerous pulse sequences, it provides information on various aspects of studied systems at the molecular level. This makes solid-state NMR an excellent technique for studying energy materials and energy storage devices such as batteries and supercapacitors, both ex-situ and in-situ.

Sodium-based technology is drawing attention due to the availability of raw materials, namely sodium being the fourth most abundant element in Earth's crust. NASICON-structured materials are attractive for electrochemical applications due to their favorable structural stability, high ionic conductivity and wide range of redox potentials.

Recent advancements in multinuclear ^{31}P, ^{23}Na, ^{51}V, ^{13}C, $^{47,49}Ti$ high-resolution and ex-situ solid-state NMR will be presented. High-resolution NMR allows for monitoring the dissolution of the ions during the GCD cycling and correlating with the electrochemical performance of $Na_{3-x}V_{2-x}Ti_x(PO_4)_3$-based electrodes. Multinuclear ex-situ solid-state NMR allows for detecting and monitoring aqueous electrochemical degradation and solid-electrolyte interphase formation. The formed interphase consists of amorphous phases similar to $TiO(OH)(H_2PO_4)\cdot nH_2O$ or $NaV_2(PO_4)_3$ for $NaTi_2(PO_4)_3$ or $Na_{2.5}V_{1.5}Ti_{0.5}(PO_4)_3$ and carboxylic groups on carbonaceous phases. The formation of these interphases leads to capacity loss during charge-discharge cycling of the $Na_{3-x}V_{2-x}Ti_x(PO_4)_3$ -based electrochemical devices.

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ACS Appl. Energy Mater. 2024, 7, 24, 11665–11669

Keywords

Sodium Batteries, aqueous degradation, ex situ NMR, solid state NMR

Acknowledgements

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Materials for Energy, Materials for Photonics, Theoretical Modeling of Functional Materials and Devices

Technologies and Devices

Positron annihilation approaches to the study of free-volume defects in functional nanostructured materials

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The specifics of applying positron annihilation lifetime spectroscopy (PALS) to the investigation of extended free-volume defects in functional nanostructured materials are demonstrated for technologically modified $MgAl_2O_4$ and $Cu_{0.1}Ni_{0.8}Co_{0.2}Mn_{1.9}O_4$ ceramics in bulk and thick-film forms, Eu^{3+}-doped $BaGa_2O_4$ ceramics, and Ge–Ga–Se(S)–CsCl chalcogenide glasses. PALS measurements were performed using an ORTEC system with a ^{22}Na positron source. The spectra were analyzed with LT software using two-, three- and four-component fitting procedures depending on structural features of the materials. Two main annihilation channels were identified: positron trapping at free-volume defects and ortho-positronium (o-Ps) annihilation in intrinsic nanopores. For $MgAl_2O_4$ ceramics [1], increasing sintering temperature leads to volume shrinkage and a reduction in defect-related voids accompanied by a decrease in nanopore size. In Eu^{3+}-doped $BaGa_2O_4$ ceramics [2], increasing Eu^{3+} concentration from 1 to 3 mol% results in agglomeration of free-volume defects and nanopore expansion, whereas higher dopant content causes fragmentation of defects and pores. In $Cu_{0.1}Ni_{0.8}Co_{0.2}Mn_{1.9}O_4$ ceramics [3], variation of NiO phase content induces transformations of internal defects associated with monolithization processes [3]. In chalcogenide glasses, crystallization of $80GeSe_2$–$20Ga_2Se_3$ during annealing [4] leads to fragmentation of larger free-volume nanovoids, while CsCl addition in GeS_2–Ga_2S_3 glasses promotes void agglomeration at ~10 mol% CsCl.

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Keywords

Positron annihilation spectroscopy, defect structure, nanostructured materials, chalcogenide glasses, spinel vceramics

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Materials for Energy, Theoretical Modeling of Functional Materials and Devices

Theoretical Modeling of Functional Materials and Devices

First principles computer modelling of advanced materials for fusion applications

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The radiation-resistant oxide insulators are important materials for optical widows of fusion reactors where radiation damage is critical issue. It is very important to predict/simulate a long-time defect structure evolution including thermal defect annealing after irradiation. For further prediction of the radiation stability of materials, it is also necessary to determine interstitial migration energy and diffusion pre-exponent. Diffusion controlled recombination of interstitials and complementary electron (F type) centers control optical and mechanical properties of oxides. We discuss multiscale computer simulations [1-4] combining the first principles calculation of the atomic, electronic, magnetic structure and optical properties of defective oxides with the kinetics of defect recombination upon annealing. We performed large scale computer calculations of basic defects and analyzed available experimental kinetics of the radiation defect annealing for three different ionic solids: neutron/ion-irradiated Al_2O_3 (sapphire), ion-irradiated $Y_3Al_5O_{12}$ (YAG), $MgAl_2O_4$ spinel and diamond -- all four wide gap insulating materials but with different crystalline structures. We demonstrate that the dependence of defect migration parameters on the radiation fluence plays an important role in the quantitative analysis of the radiation damage of real materials and should not be neglected.

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Keywords

radiation defects; functional materials, first principles calculations, defect annealing

Acknowledgements

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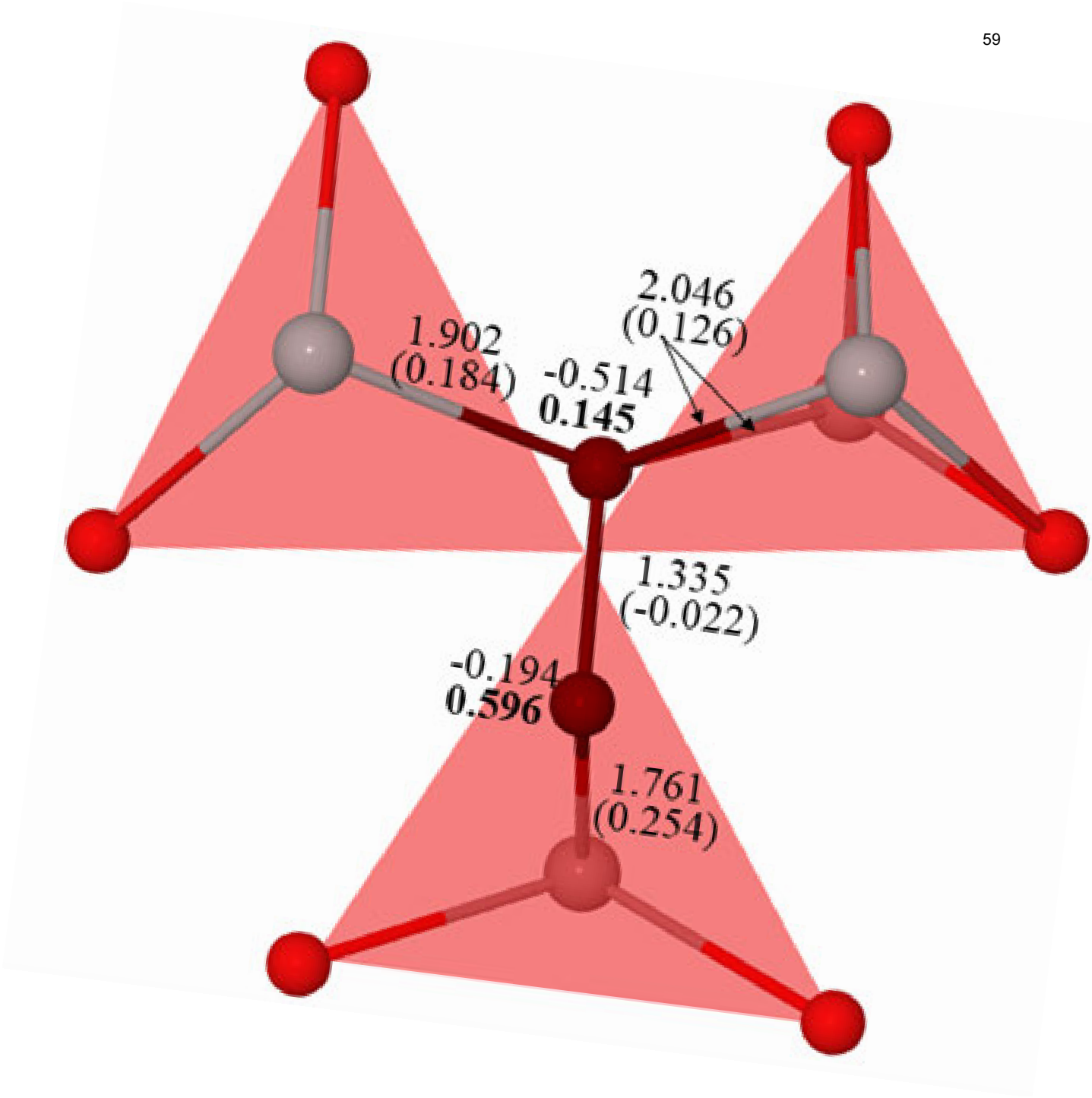
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1.761
(0.254)

Technologies and Devices, Large-Scale Research Infrastructures, Science Policy and Collaboration

Large-Scale Research Infrastructures & Science Policy

X-ray absorption spectroscopy study of polycrystalline V1-xRexO2 solid solution

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Julija Lukasevica , Institute of Solid State Physics, University of Latvia, Riga, Latvia
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Edmund Welter , Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Vanadium dioxide (VO_2) is a well-known and intriguing “smart” material that exhibits a reversible hysteretic-type metal-to-insulator transition (MIT) between the low-temperature monoclinic VO_2(M1) and high-temperature tetragonal VO_2(R) phases at T_C ~ 68 °C [1]. Substitutional, interstitial, charge, or chemical doping of VO_2 can significantly affect the transition temperature [2].

While numerous chemical elements have been investigated as dopants to control the MIT temperature in VO_2 [2], only a few studies have been dedicated to rhenium [3, 4]. In the $V_{1-x}Re_xO_2$ solid solution, increasing the rhenium content to x = 0.10 drastically lowers T_C by about 80 °C [4]. Moreover, the presence of rhenium ions in the +6 oxidation state was suggested at low concentrations (x <= 0.03) based on XPS data [4].

In this study, the local structure of the $V_{1-x}Re_xO_2$ (x = 0.01-0.15) solid solution was investigated using in situ X-ray absorption spectroscopy at the V K-edge and Re L_3-edge over the temperature range 80-420 K. The dependence of the MIT on rhenium content was confirmed from by analysis of the V K-edge XANES and EXAFS spectra and supported by density functional theory calculations. The peculiarities of the local environment in the M1 and R phases were determined using reverse Monte Carlo simulations [5] of the V K-edge EXAFS spectra. Strong distortions of the first coordination shell of rhenium atoms were also observed at low rhenium content (x <= 0.03).

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Keywords

V1-xRexO2 solid solution, X-ray absorption spectroscopy, reverse Monte Carlo simulations

Acknowledgements

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Hot electrons in plasmonic nanoparticles: from creation to catalysis

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Localized surface plasmons in metallic nanoparticles give rise to very strong light absorption. The decay of these excitations results in the generation of energetic or “hot” electrons and holes which can be harvested and harnessed for applications in photovoltaics, photocatalysis and sensing. To optimize hot carrier production in devices, a detailed theoretical understanding of the relevant microscopic processes, including light-matter interactions, plasmon decay and hot electron thermalization, is needed. In my talk, I will describe a material-specific theory of hot-carrier generation and relaxation in metallic nanoparticles which combines a classical description of the electromagnetic radiation with large-scale atomistic quantum-mechanical simulations. I will present results for hot carrier distributions in spherical nanoparticles of gold, silver and copper and discuss the relative importance of interband and intraband transitions as function of nanoparticle size. Next, I will describe how CO2 reduction performance of gold nanoparticles can be enhanced by changing the nanoparticle shape. Finally, I will present results for bimetallic Au-Pd photocatalysts and demonstrate a large enhancement in hydrogen production can be achieved in antenna-reactor architectures.

Single crystal growth of functional materials at NCKU

CHIN SHAN LUE , National Cheng Kung University

Chia Nung Kuo , National Cheng Kung University

I will introduce to the Taiwan Consortium of Emergent Crystalline Materials (TCECM), supported by National Science and Technology Council (NSTC) and my crystal growth laboratory at National Cheng Kung University (NCKU). Up to now, we have successfully synthesized over two hundred kinds of single crystalline compounds using diverse techniques. Our crystals cover a wide range of material systems including novel superconductors, emergent topological materials, layered magnetic systems, and multifunctional 2D materials. I will also discuss various investigations of these crystals via domestic and international collaborations.

Keywords

Single crystal growth, Functional materials, Quantum Materials

Protons in mixed-conducting perovskites: Why, how many, and how fast?

Rotraut Merkle , Max Planck Institute for Solid State Research

Triple-conducting oxides such as $BaFeO_3$ as containing mobile oxygen vacancies, protons, and electronic defects are key functional materials, e.g. for air electrodes in protonic ceramic fuel cells The proton conductivity is decisive to activate the whole electrode surface for the oxygen reduction to water.

Proton uptake occurs through hydration or hydrogenation, depending on material and conditions.[1] Triple-conductors typically show less hydration than $Ba(Ce,Zr,Y)O_{3-z}$ electrolyte materials. Experiments and DFT+U calculations indicate that the high covalency of the Fe-O bonds decreases the basicity of the oxide ions.[2,3] Proton conductivity and mobility in $BaFeO_{3-d}$ is determined from chemical diffusion and isotope exchange experiments.[4]

DFT+U calculations of $BaFeO_{3-d}$show that the proton transfer begins with an approach of donating and receiving oxygen, followed by O-H bond breaking.[5] Thus, the O-O distance is decisive for the proton transfer. The proton migration barrier of ≈0.2 eV is significantly lower than for oxide ions. Fe-site dopants such as Ga^{3+},Sc^{3+},In^{3+},Y^{3+} cause lattice distortions and defect interactions. The strongly oversized Y^{3+} even repels protons from its first coordination shell.[6] Overall, a comprehensive picture of proton uptake and mobility is derived, which can be employed in further materials optimization.

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Keywords

Proton-conducting oxides, protonic ceramic fuel/electrolysis cells, defect chemistry, DFT calculations

EuroNanoLab: present and future of the European distributed research infrastructure on micro- and nano-fabrication

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As reported in the ESFRI Landscape Analysis 2024 [1], to maintain the EU leadership role in the technology development in several different sectors like photonics, advanced materials, nanotechnology, micro and nanoelectronics, and advanced manufacturing technologies **there is the need of a global management of nanofabrication processes on an EU-scale, to enable and promote a better use of present and future resources, provide open access to nanofabrication technologies, instruments knowledge & training, reduce the access time to the desired technology, and therefore accelerate research in many different fields**.

In the last years, to face these challenges, EuroNanoLab (ENL) [2] has **established a pan European research infrastructure** in the field of nanofabrication by **clustering and organizing already existing academic nanofabrication infrastructures** on an EU scale. By consolidating **academic nanofabrication centres**, services, and core resources into a coordinated nanofabrication infrastructure, ENL aims at **supporting the fabrication-related needs of about 10.000 scientists** through open-access to **nanofabrication instruments, expertise, services and training existing in EU academic cleanrooms.**

Present organization of ENL, ongoing activities, collaborations at the EU and at the international level [3], the actual and possible future impacts on National strategies, as well as future perspectives in terms of integration of the nodes, engagement of the users' communities, services to scientific communities and private stakeholders as well as integration in the European Research Area and Research and Technological Infrastructures will be presented.

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[1] ESFRI Landscape Analysis 2024 - https://landscape2024.esfri.eu/ [2] https://euronanolab.eu/ [3] https://globalnanolab.org/

Keywords

nanofabrication, technology, research infrastructure, technological infrastructure

Deposition of ZnO-Ga2O3 and Ir2O3-Ga2O3 thin films by reactive co-sputtering of liquid gallium

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Edgars Butanovs , Institute of Solid State Physics, University of Latvia
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Thin films of Ga_2O_3 and $ZnGa_2O_4$, as well as solid solutions Ir_2O_3-Ga_2O_4 are of technological interest due to their applications in wide bandgap electronic and optoelectronic devices. We have developed a method for reactive liquid magnetron sputter deposition of gallium oxide thin films [1]. In this study, we report the deposition amorphous and crystalline thin films of Ga_2O_3 [2] and $ZnGa_2O_4$ [3] by reactive pulsed direct current magnetron sputtering from a liquid gallium target onto fused quartz and c plane sapphire substrates, where the temperature of the substrate is varied from RT to 800°C. Non-stoichiometric $ZnGa_2O_4$ thin films, covering a wide range of Ga:Zn atomic ratios (≈ 0.3 – 5.7), were deposited by co-sputtering solid Zn target next to liquid Ga target. The composition was controlled by varying the sputtering power of the Zn target and monitoring the process with plasma optical emission spectroscopy. Composition analysis shows no traces of impurities and a slight oxygen deficiency in the films. The static deposition rate of Ga_2O_3 (up to 37 nm/min at RT on f-quartz and 5 nm/min at 800 °C on c-sapphire) is two to five times higher than the rates reported in the literature for radio frequency sputtering. When deposited onto unheated substrates, the films are X-ray amorphous. Well-defined X-ray diffraction peaks of β-Ga_2O_3 begin to appear at a substrate temperature of 500°C, and $ZnGa_2O_4$ peaks at 300°C. Electron microscopy images reveal a dense and void-free microstructure. The thin films are highly transparent in the visible light range (≈ 84%) and the optical band-gap varies between approximately 3.9 eV and 5.1 eV, depending on the amount of Zn in the composition.

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Keywords

Wide bandgap semiconductors, Ga_2O_3 , $ZnGa_2O_4$, Sputtering

Microfluidic PDAC-on-a-Chip for Patient-Specific Drug Testing

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Vadims Parfejevs , University of Latvia
Kaspars Jekabsons , University of Latvia
Liga Kunrade , University of Latvia
Kristaps Klavins , Riga Technical University
Ilva Trapina , University of Latvia
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Una Riekstina , University of Latvia

Pancreatic ductal adenocarcinoma (PDAC) is characterized by high mortality and limited therapeutic options. Standard-of-care systemic regimens, depending on tumor stage and patient performance status, include FOLFIRINOX (folinic acid, 5-fluorouracil, irinotecan, oxaliplatin) and gemcitabine plus nab-paclitaxel, whereas gemcitabine monotherapy is generally reserved for patients with poor performance status (1). To improve outcomes, there is a critical need for tumor markers enabling early detection, response assessment and targeted therapies based on molecular tumor profiling. Advanced *in vitro* models, such as organoids and organ-on-chip systems, are emerging to help bridge this gap and support clinical decision-making. We established a library of patient-derived, treatment-naive PDAC organoids and developed a PDAC-on-chip model with vascular and tumor channels to recapitulate key features of the tumor microenvironment and study intratumoral drug distribution and antitumor effects in a patient-specific context (2). Using this chip, we show that gemcitabine and SN-38 at clinically relevant plasma concentrations exert only limited cytotoxic effects on PDAC cells compared with conventional static 2D and 3D cultures. These data indicate that the PDAC-on-chip model enables drug sensitivity testing under physiologically relevant conditions and supports its further evaluation as a functional precision medicine tool in PDAC.

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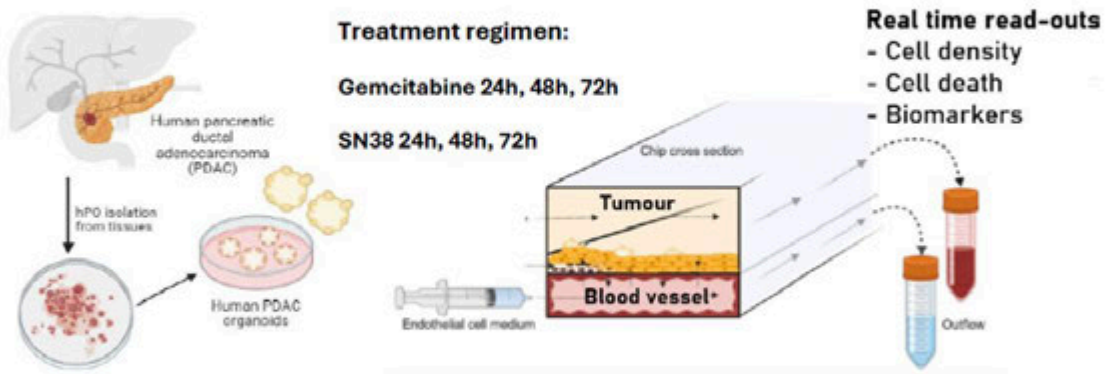
Keywords

Pancreatic ductal adenocarcinoma; Patient-derived organoids; Microphysiological systems; Functional precision oncology

Acknowledgements

Postdoc Latvia Nr. 1.1.1.9/LZP/1/24/163 “Preserving pancreatic tumour complexity in zebrafish xenografts for precision oncology” Latvian Science Council grant lzp-2024/1-0206 "Targeting pancreatic ductal adenocarcinoma-on-a-chip with aptamer-guided extracellular vesicle delivery"



Emergence of a relaxor phase and dimensional tuning in mixed 2D hybrid perovskites

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Gabrielius Rimkus , Vilnius University
Sergejus Balciunas , Vilnius University
Anna Gagor , Institute of Low Temperature and Structure Research, Polish Academy of Sciences
Daria Szewczyk , Institute of Low Temperature and Structure Research, Polish Academy of Sciences
Katarzyna Fedoruk-Piskorska , University of Silesia in Katowice
Jan K. Zareba , Wroclaw University of Science and Technology
Adam Sieradzki , Wroclaw University of Science and Technology
Vytautas Klimavicius , Vilnius University
Juras Banys , Vilnius University
Miroslaw Maczka , Institute of Low Temperature and Structure Research, Polish Academy of Sciences
Mantas Simenas , Vilnius University

Mixing of molecular cations in hybrid lead halide perovskites offers a powerful route to tailor their optoelectronic functionality, structural stability, and phase-transition behavior. While such compositional engineering has been extensively studied in three-dimensional perovskites, its impact on low-dimensional analogues remains largely unexplored. Here, we investigate cation-mixing effects in the Ruddlesden-Popper $BA_2MA_{n-1}Pb_nBr_{3n+1}$ two-dimensional perovskites using a comprehensive multitechnique approach.We show that substituting methylammonium (MA) with dimethylammonium (DMA) transforms the long-range ferroelectric phase into a state characterized by frustrated electric dipoles. Broad-band dielectric measurements reveal that this state is a relaxor phase, previously unobserved in three-dimensional hybrid perovskites. Remarkably, cation mixing also governs perovskite dimensionality enabling stabilization of thick-slab members up to n = 5 in single-crystal form. These results establish cation mixing as a versatile tool to control both polar order and dimensionality in two-dimensional hybrid perovskites.

Keywords

hybrid perovskite, relaxor, phase transition

Acknowledgements

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Hybrid SALD–PVD approaches for electron contact layers in perovskite/silicon tandem solar cells

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Sven Pleger , Fraunhofer IST
Christian Beyen , Fraunhofer IST

Perovskite/silicon tandem solar cells require electron contact stacks that combine excellent interface passivation with scalable, low-temperature processing. In this work, we present a hybrid coating platform that unites spatial atomic layer deposition (SALD) with thermal physical vapor deposition (PVD) in a single vacuum-integrated tool. The system enables sequential deposition of AlOx/C60/SnOx electron contact stacks on large-area substrates compatible with G12 wafer formats. A custom linear C60 evaporator was designed and optimized using Direct Simulation Monte Carlo (DSMC) modelling and subsequently validated by large-area thickness and absorption mapping, demonstrating high uniformity of the hybrid-deposited layers. Integrated single-wavelength ellipsometry provides real-time thickness control and reveals a pronounced nucleation delay for SnOx growth on hydrophobic C60, which is critical for process integration. Overall, the results demonstrate that hybrid SALD–PVD processing offers a viable and industry-relevant route towards scalable electron contact architectures for next-generation perovskite/silicon tandem solar cells.

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Volker Sittinger et al. Surface & Coatings Technology 522 (2026) 133150

Keywords

Perovskite/silicon tandem solar cells; hybrid SALD–PVD; AlOx/C60/SnOx; large-area deposition; inline ellipsometry; passivation; electron contact stack

Acknowledgements

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Materials for Energy, Large-Scale Research Infrastructures, Science Policy and Collaboration

Large-Scale Research Infrastructures & Science Policy

X-ray absorption spectroscopy as an advanced characterization tool for compositionally complex systems

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Compositionally complex systems are represented by a broad class of materials, and are already recognized as being promising for practical applications in renewable energy technologies, catalysis, battery research, or as coatings under extreme conditions like temperature, mechanical stress and radiation. These systems traditionally include high-entropy alloys (HEAs), high-entropy oxides (HEOs), high-entropy carbides (HECs), *etc*, and exhibit many extraordinary properties due to their extremely high atomic heterogeneity achievable through a number of different components. Unveiling the roles of individual constituents in the structural, electronic, and magnetic properties of compositionally complex systems is of key importance for further developments in materials science, and makes X-ray absorption spectroscopies available at different synchrotron radiation facilities even more demanding. Nowadays, a plethora of unique characterization tools can be found for advanced element-specific studies at the atomic scale due to energy tunability, variable polarization, high flux and time structure of synchrotron X-ray photons.

In this talk, the benefits of multi-edge extended X-ray absorption fine structure (EXAFS) spectroscopy in combination with reverse Monte-Carlo (RMC) simulations, X-ray magnetic circular dichroism (XMCD) spectroscopy performed in pulsed magnetic fields and X-ray photoemission electron microscopy (X-PEEM) in application to HEAs studies [1-7] will be highlighted.

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Keywords

EXAFS, RMC, XMCD, XPEEM, HEAs

Acknowledgements

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Advances in Microfluidic Electrochemical Biosensors for Microbial Biofilm Analysis

Arunas Stirke , Center for Physical Sciences and Technology (FTMC)

Microbial biofilms play a critical role in infections and antibiotic resistance, necessitating advanced methods to comprehensively study their behavior across diverse environments. Electrochemical biosensors, particularly when integrated with microfluidic technology, have revolutionized the detection and real-time analysis of biofilm dynamics, virulence, and properties, offering heightened sensitivity and precision. Recent advancements include the development of graphene-based field-effect transistor (G-FET) biosensors within custom microfluidic platforms for rapid and ultra-sensitive detection of pathogens such as SARS-CoV-2 and its variants, utilizing recombinant ACE2 as the binding receptor. These platforms enable detection at attogram levels and demonstrate selectivity against related viral proteins, underscoring their transformative potential for both fundamental biofilm research and clinical diagnostics. This review critically examines the properties, advantages, and applications of microfluidic electrochemical biosensors, highlighting their promise in advancing our understanding of microbial biofilms and facilitating early diagnosis and monitoring of infectious diseases.

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https://doi.org/10.1021/acsomega.5c04643, https://doi.org/10.3389/fcimb.2024.1419570

Keywords

Microfluidic biosensors, Electrochemical detection, Microbial biofilm analysis and Graphene-based sensors

Nanostructured Materials for Silicon Photovoltaics

Pauls Stradins , National Laboratory of the Rockies

In this talk, I review the fundamental and technological limitations of industrially relevant PV technologies, focusing of the Si PV that leads the PV worldwide. Then, I highlight nanotechnologies that enable multiple aspects of high-performance Si solar cells. In particular, I discuss three ways to create nanopinhole-enabled, high performance passivated carrier-selective contacts to Si cells: metal-assisted nano corrosion; self-assembled monolayers, and engineered laser nano ablation.

Substrate-controlled point defects in thin films of perovskite oxides

Marina Tyunina , University of Oulu (Finland); Institute of Physics (Czechia)

ABO_3-type perovskite transition-metal oxides constitute a broad class of multifunctional materials with electronic properties ranging from insulating to superconducting and exhibiting diverse charge, spin, and polar orders. In the last decades, research of perovskite oxide thin films has yielded fascinating discoveries. In parallel, the global expansion of perovskite oxide ferroelectric thin-film synthesis and applications has revealed significant variability and poor reproducibility in films' behavior. While leading researchers often attribute this scatter to imperfect synthesis and call for improved growth techniques, such variability may also indicate that fundamental thin-film effects remain insufficiently understood.

In the presentation, it will be shown that point defects which are difficult or impossible to directly probe experimentally in thin films - can be controlled by substrates. As a result, anomalous lattice strain and unconventional dielectric and charge-transport behavior may emerge in thin films. The archetypal perovskite oxide $SrTiO_3$ is used as the primary model system, with additional proofs drawn from titanates, niobates, and nickelates. Experimental thin-film growth by pulsed laser deposition and multimodal characterization are combined with multiscale modeling.

Electrochromic materials for visible and near infrared light modulation

Ruitao Wen , Southern University of Science and Technology

Electrochromic materials can reversibly change their optical properties by varying the external electrical stimuli. Since the first experimental demonstration of electrochromic phenomenon in tungsten oxide, electrochromic technology has been extensively developed. Currently, electrochromism based devices can be found in windows of energy efficient buildings, smart phones, goggles, information displays, anti-glare rear-view mirrors, etc. In inorganic electrochromic materials, transition metal oxides are most studied, and oxide thin films can change colors and transmittance of the near-infrared between a transparent and a colored state upon small ion intercalation. In an electrochromic material or device, an ideal scenario is that visible and near-infrared light can be independently regulated, that is *bright* mode (both VIS and NIR are highly transparent), *cold* mode (transparent for VIS but not for NIR), warm mode (transparent for NIR but not for VIS) and dark mode (both VIS and NIR are blocked). However, electrochromic devices typically suffer from single-mode control, *i.e.*, simultaneously varying the visible and near-infrared light. Electrochromic effect combined with surface localized plasma resonance (LSPR) were recently found to be able to sequentially modulate near-infrared and visible light. In this talk, we report our recent progress on dual-band modulation, with a special focus on achieving a transition from *bright* mode to *warm* and *dark* mode, as well as *bright* mode to *cool* and *dark* mode. We believe our findings show substantial fundamental insight into electrochromism in cathodic oxides, and provide a new starting point for designing electrochromic devices with superior performance.

ABSTRACTS

of the ORAL PRESENTATIONS

Alphabetically by Corresponding Authors

Hybrid Metal Oxide Nanowires for Bias-Free Photo-Driven Simultaneous Energy Generation and Carbon Dioxide Reduction

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This work reports a proof-of-concept for the simultaneous bias-free generation of electrical power and reduction of carbon dioxide into value-added hydrocarbons from a humid gaseous environment under simulated solar irradiation, using advanced CuO-Cu_2O-ZnO hybrid nanowire arrays. Free-standing hybrid nanowire arrays were directly grown on a copper substrate through a simple, reproducible fabrication route combining thermal oxidation and low-pressure physical vapor deposition. Under simulated solar illumination, the CuO-Cu_2O-ZnO hybrid nanowire arrays operated in a CO_2-saturated atmosphere with a relative humidity of approximately 50%, enabling the simultaneous generation of electrical output in the range of several nW/cm^2 and photocatalytic conversion of CO_2 into methane, ethylene, and methanol. The artificial photosynthesis process proceeded with a conversion rate of about 2.2 μmol/cm^2·h and was accompanied by an increase in the O_2 content of the surrounding environment by up to 20%, while relying solely on simulated solar light as the external energy source. The observed self-powered photothermoelectric and photocatalytic performance is attributed to efficient separation of photogenerated charge carriers within cascading type-II heterojunctions, which create multiple built-in electric fields and promote self-driven charge separation throughout the hybrid structure. In addition, the high surface area of nanostructured ZnO provides abundant active sites for CO_2 adsorption and subsequent reduction. These findings highlight the potential of CuO-Cu_2O-ZnO hybrid nanowire arrays as environmentally friendly, metal oxide-based multifunctional platforms for solar energy harvesting

and CO_2 conversion, opening new opportunities for the development of energy-efficient and carbon-neutral devices and coatings.

Keywords

zinc oxide; copper oxide; hybrid nanowire; carbon dioxide reduction; photo-driven energy generation

Acknowledgements

This work was performed within the Latvial Council of Science funded Fundamental and Applied Research project No. lzp-2022/1-0239 «Multifunctional hybrid metal oxide nanowire arrays for simultaneous green generation and CO2 reduction».

ENHANCED THERMAL STABILITY IN GRAPHENE-BASED GAS SENSORS THROUGH THIN ANTIMONY OXIDE FILMS

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Margus Kodu , Institute of Physics, University of Tartu
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Raivo Jaaniso , Institute of Physics, University of Tartu

In recent years, graphene has emerged as a compelling platform for next-generation gas-sensing technologies, owing to its remarkable electronic properties and atomically thin structure. However, the inert nature of graphene in its pristine form limits its use as both a receptor and a transducer in chemiresistor gas sensors. It has been shown that incorporating a functional layer, such as metals or metal oxides [1,2], atop graphene to serve as a receptor can markedly enhance its sensing toward a range of toxic and pollutant gases. Nevertheless, such functionalized sensors are often prone to face a sensitivity-stability trade-off stemming from surface modification, making them vulnerable to degradation, especially in high-temperature and long-term operations.

In this work, we demonstrate, for the first time, a protective effect of thin antimony oxide films deposited on graphene gas sensors via pulsed laser deposition. We show that graphene sensors can detect CO gas only when functionalized with Pt, but a dramatic degradation occurs when heating above 200 °C. However, intercalation of a thin antimony oxide enables the sensor to withstand the high temperature, without losing its sensitivity to CO gas. This protective effect is highly reproducible, and the enhanced stability is maintained for at least 2 years, highlighting antimony oxide as a promising material for addressing the long-standing stability challenge in sensor research.

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Keywords

Graphene, Antimony oxide, Chemiresistors, Pulsed laser deposition

Acknowledgements

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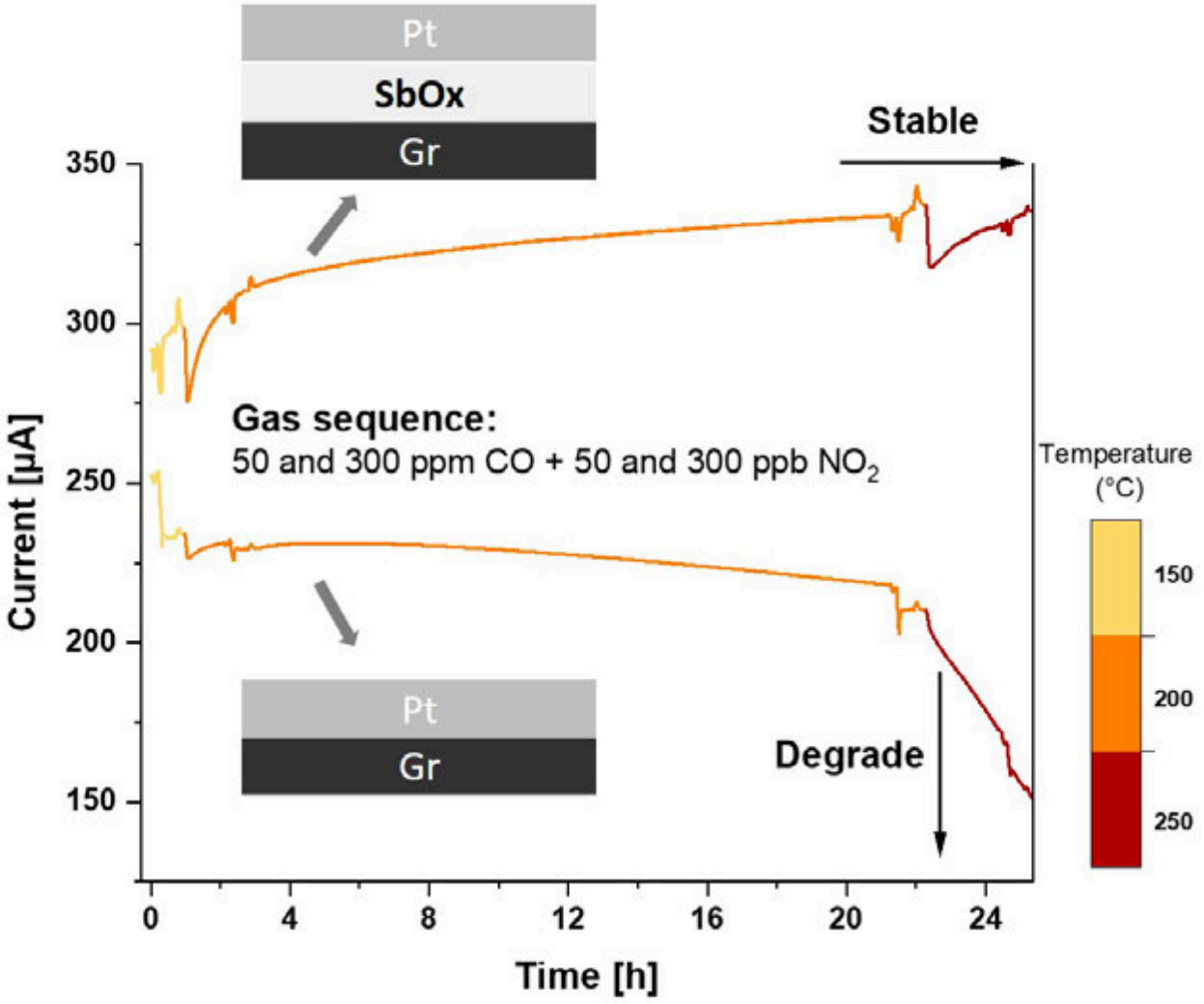


Fig.1 Sensor responses to CO and NO_2 at elevated temperatures. Above 200 °C, the sensor with an antimony oxide layer remains stable, whereas the unprotected sensor shows a significant current drop, indicating degradation.

Turning Strategy into Practice: SWOT Analysis for Integring Microfluidic Rapid DNA Technologies

Amit Blumberg , ordnary

Noam Shomron , Gray Faculty of Medical and Health Sciences, Tel Aviv University, Tel Aviv, Israel

The integration of microfluidic rapid DNA technologies into forensic identification workflows requires not only advanced instrumentation but also a structured strategic framework. This study demonstrates how SWOT (Strengths, Weaknesses, Opportunities, Threats) analysis can guide the effective integration of microfluidic systems into large-scale forensic operations. The approach was implemented following the October 7, 2023 mass fatality incident in Israel, where the Israel Defense Forces Genomic Center for Casualties Identification expanded its operational capacity to address an unprecedented identification challenge involving fragmented and degraded human remains.

Conventional identification methods were often unavailable, making DNA profiling the primary identification tool. Microfluidic rapid DNA systems enabled genetic profiles to be generated within approximately 2–3 hours. However, operational experience showed that successful implementation depended on structured SWOT-based evaluation that guided workflow design and sample prioritization.

The analysis identified key strengths including speed, automation, and deployability; weaknesses such as sensitivity to sample quality and throughput limitations; opportunities for improved preparedness and decentralized forensic capability; and threats related to logistical and validation challenges.

These findings demonstrate that SWOT analysis provides an effective operational framework for integrating microfluidic rapid DNA technologies and offers a practical model for future mass fatality response

Exploring ferroelectric and electrical properties in Cobalt Doped BiFeO3 prepared via modified chemical solution method

Yevhen Brych , University College Dublin

Waseem Wani , University College Dublin

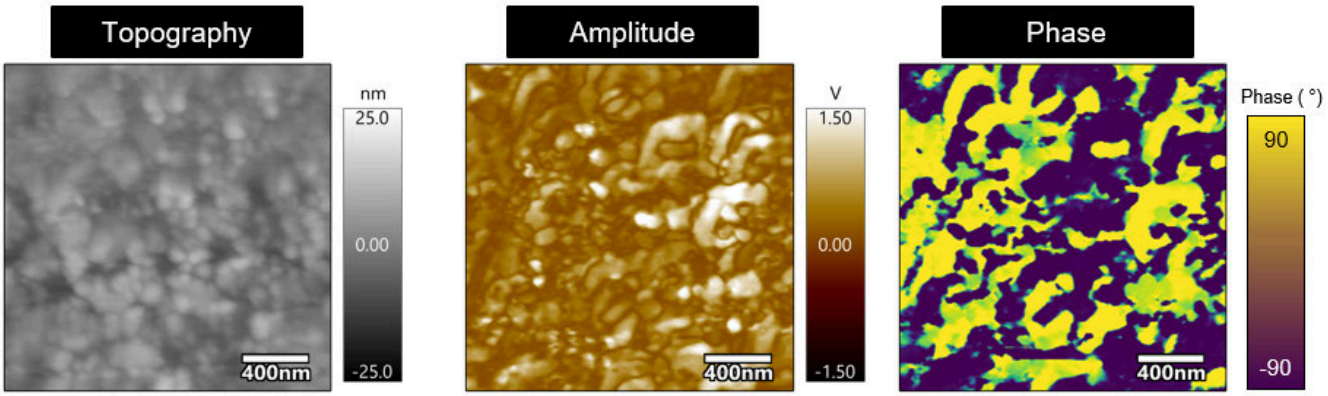
This work investigates BFO thin films prepared via the sol–gel method, which can produce high-quality films suitable for functional applications. The composition of these films was verified with EDS and cross-sectional SEM data to confirm the BFO/ITO/glass stack structure. The surface topography was examined by atomic force microscopy, revealing an average surface roughness of 4 ± 2 nm. Vitally, XRD confirmed the presence of the pure BFO phase. In addition, the sample was doped with cobalt, the presence of which was identified in the EDS spectra. Optical band gap measurements revealed that cobalt doping reduces the band gap. Additionally, J–V curve analysis indicated a linear response over a wide electric field range, suggesting a reduced trap-state effect. Despite a high leakage current due to cobalt doping, PFM studies were used to successfully measure the ferroelectric response of the film, with a clear 180° phase difference observed (See figure 1). Further PFM-based investigations such as Vac sweeps confirmed ferroelectricity, with the first harmonic being higher than the second harmonic. BEPS hysteresis loops also showed a clear ferroelectric response with a coercive voltage of approximately 5 V and minimal imprint. Finally, the local electrical properties of the sample were investigated using C-AFM and KPFM to map the heterogeneous conductivity and surface potential of the film.

Keywords

Ferroelectrics, AFM, Doping

Acknowledgements

This work was primarily performed by Dr Waseem Wani. Due to circumstances Yevhen Brych (a minor contributor) will be presenting it.



Polymer Photonics for Highly Nonlinear Host-Guest System Integration in Photonic Integrated Circuits

Arturs Bundulis , AP4PIC

As integrated photonics start to play more essential role in telecommunications, data centers and quantum technology, Photonic integrated chip (PIC) fabrication becomes a more competitive environment with each new technology promising lower energy consumption, smaller footprint and wider application range. Polymer-based photonic platform offers a unique approach to efficiency and production cost. Possibility to create host-guest systems allows to integrate highly nonlinear optical dyes, decreasing the threshold power of frequency comb generation or quantum light sources by order of magnitude. At the same time wet-coating production flow allows for cheaper PIC fabrication cost.

In this work we focus on two key aspects of polymer platform – nonlinear optical (NLO) dye research and two-step lithography process for ring resonator structure formation. Studied organic dyes reach Kerr coefficients of 10^{-15} - 10^{-16} m^2/W. The selected organic dyes were also tested for UV stability. For two step lithography process direct laser writing was employed for dye systems stable under UV exposure, enabling flexible and high-resolution structuring of polymer photonic components. This allowed to reach <400 nm gap size between waveguides and ring resonator structures.

Keywords

Nonlinear optics, photonics, optical lithography

Materials for Photonics, Large-Scale Research Infrastructures, Science Policy and Collaboration

Large-Scale Research Infrastructures & Science Policy

Optimization of Sol–Gel Synthesis Parameters for $LaAlO_3$ Nanoparticles and Their Impact on Luminescence Properties

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Aleksei Kotlov , Deutsches Elektronen-Synchrotron DESY
Alina Popova , V. N. Karazin Kharkiv National University
Tetiana Voitenko , University of Cambridge
Luiz Jacobsohn , Clemson University
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Lanthanum aluminate perovskite, $LaAlO_3$ (LAP), has a wide range of applications primarily based on the excellent properties of its bulk crystals. Owing to its flexible perovskite structure and wide band gap, LAP is also considered a promising host material for luminescent activator ions. But the design of doped materials with predictable optical properties requires a detailed understanding of intrinsic emission processes of the host. However, reports on LAP host emission remain limited and vary significantly depending on synthesis conditions [1-3]. The use of high-energy photon sources, which enable excitation of excitonic and band-to-band transitions, can provide deeper insight into the actual mechanisms. In the presented work, synchrotron excitation from the DESY PETRA III Beamline P66 was used for this purpose. We targeted LAP nanoparticles synthesized via a sol–gel route given the ability of this synthesis method to manipulate polymorphism and used single crystals as references. The effects of heat treatment temperature and time on phase formation processes, crystallographic parameters, and crystallite sizes were investigated. Optimal temperature-time conditions to obtain single-phase LAP nanoparticles were determined. The emission spectra of the LAP matrix exhibit a broad band centered at around 420 nm at room temperature. The excitation spectrum of this emission shows a maximum at 220 nm, close to the band-gap edge. The matrix emission is weak in single-crystal LAP, whereas it becomes more intense in nanoparticle form. Analysis of the luminescence decay curves revealed emission lifetimes characteristic of excitonic recombination, in good agreement with the excitation band location near the fundamental absorption edge.

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Keywords

sol-gel nanoparticles, oxide perovskite, luminescence

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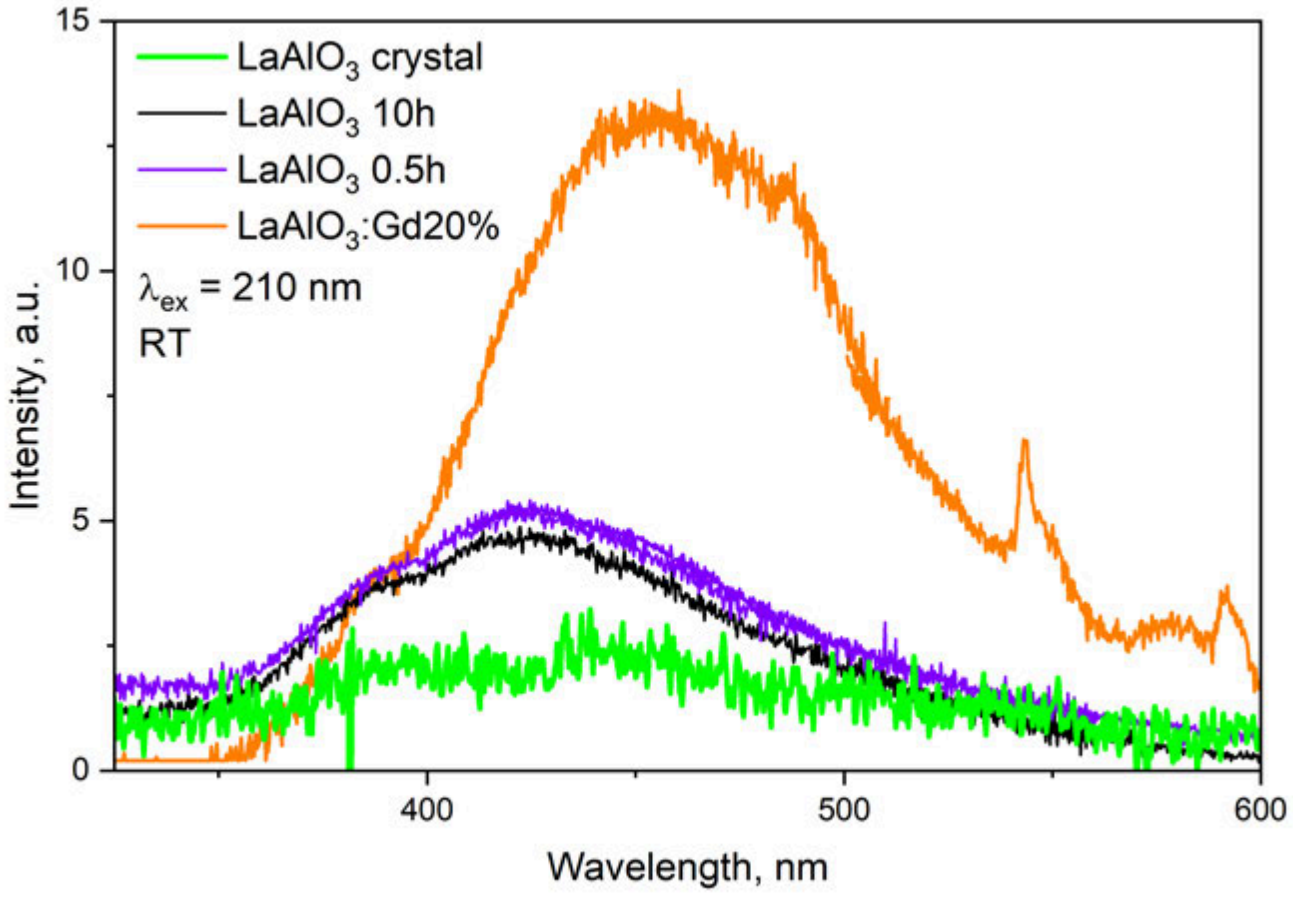

Emission from bismuth quantum dots formed in annealed GaAsBi quantum wells

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Near-infrared (NIR) semiconductor lasers are essential for optical communications, sensing, and medical technologies, motivating the search for new material systems with efficient emission in the 1.3–1.5 μm spectral range. Recently, bismuth-containing III–V compounds have attracted significant interest. Moreover, post-growth annealing of GaAsBi can lead to the formation of Bi quantum dots (QDs) exhibiting even more redshifted emission [1].

In this work, GaAsBi/(AlGa)As quantum well (QW) structures with rectangular and parabolic barriers were grown by molecular beam epitaxy and subsequently annealed at temperatures above 600 °C to induce Bi QD formation. The influence of QW design, well thickness, and barrier composition on the formation of QDs and their optical properties was investigated. Structural and optical characterization was performed using X-ray diffraction, transmission electron microscopy, photoluminescence (PL), and photoreflectance spectroscopy.

A pronounced PL band at ~0.9 eV was attributed to emission from Bi QDs formed during thermal treatment. The emission energy shows negligible shift in the temperature range from 4 to 300 K. At the same time, the intensity and thermal quenching behavior of the PL strongly depend on the QW design and growth conditions. In particular, the emission properties were found to be highly sensitive not only to the annealing process but also to the temperatures used during the growth of layers above the GaAsBi region. These results highlight the critical role of growth and thermal processing in controlling Bi QD formation and emission efficiency, providing important guidelines for the design of GaAsBi-based nanostructures for NIR optoelectronic devices.

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Keywords

GaAsBi, Bi quantum dots, photoluminescence, near-infrared

Acknowledgements

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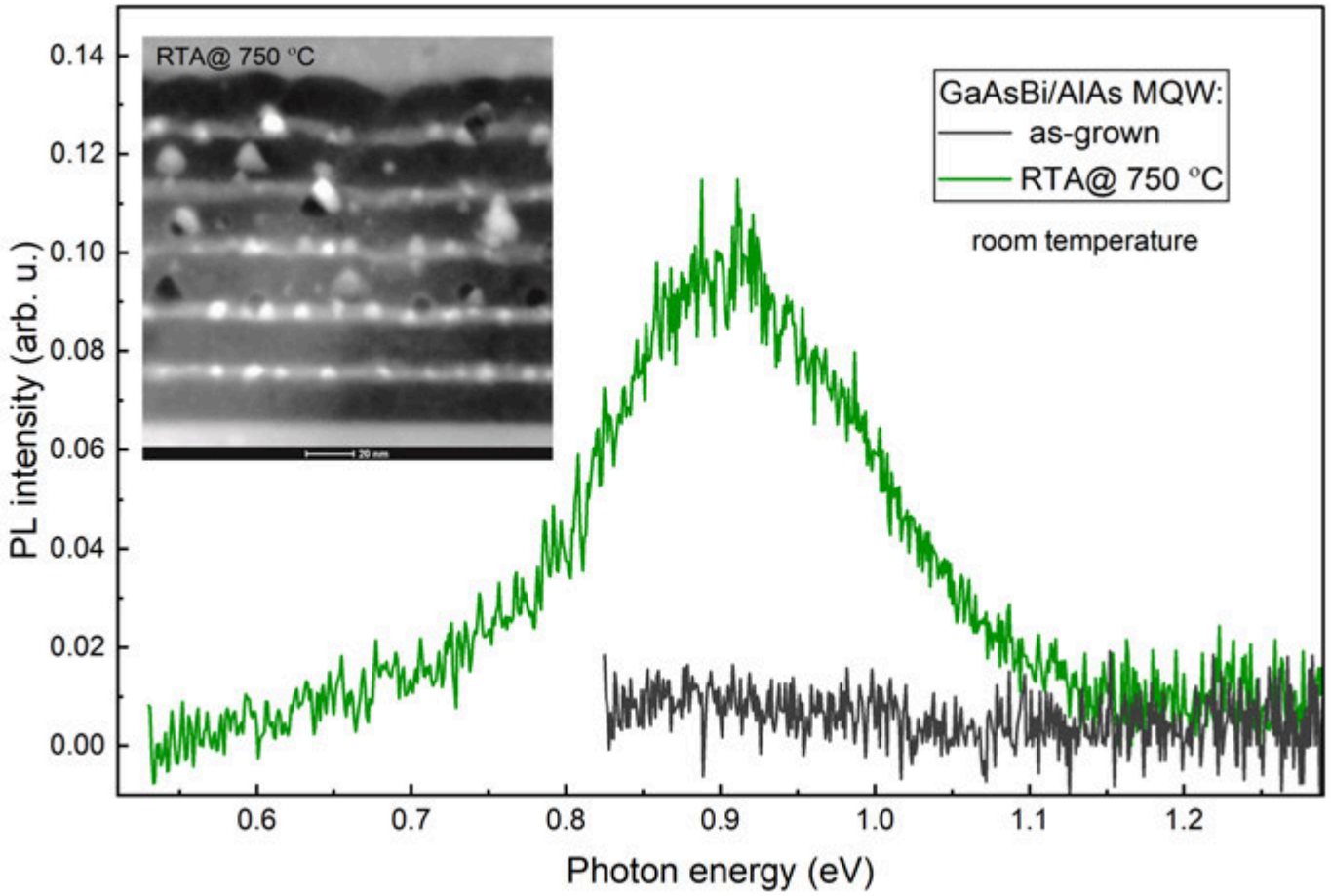

Full-spectrum Principal Component Analysis-polynomial calibration-for the high-accuracy luminescence thermometry with Eu3+/Dy3+ co-Doped La2O2S

Ljubica Đačanin Far , Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade

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Non-contact optical temperature sensing based on luminescence thermometry is a powerful and versatile approach for applications that demand high spatial and temporal resolution and the ability to operate in extreme or hard-to-reach environments [1]. Lanthanum oxysulfide is a wide band gap semiconductor widely used in the steel industry, catalysis, and electroluminescent devices. When doped with various rare-earth ions, it serves as an efficient host material for diverse phosphor applications [2]. Luminescence thermometry commonly relies on a small subset of spectral observables (e.g., intensity ratios, band shifts, etc.), which can limit accuracy when temperature induces complex, distributed changes in photoluminescence spectra. Here we present a deployable full-spectrum thermometric method for $La_2O_2S:Eu^{3+},Dy^{3+}$ based on principal component analysis (PCA) followed by low-order multivariate regression. Emission spectra acquired in the 300-700 K range (380-680 nm, 0.5 nm sampling) were area-normalized to suppress global intensity scaling, mean-centered, and decomposed using singular value decomposition. We benchmarked multiple regression families using leave-one-out cross-validation (LOOCV). After identifying the 300 K spectrum as a high-leverage outlier for prediction, we excluded it and obtained a quadratic calibration in (PC1, PC2, PC3), achieving LOOCV RMSE = 1.88 K and maximum absolute error = 3.10 K over the 325–700 K range (n = 16). We provide the explicit calibration equation, analytic expressions for differential sensitivity, and a step-by-step pipeline for computing PC1–PC3 for new spectra, enabling direct use as an optical temperature sensor.

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Keywords

Luminescence thermometry; principal component analysis; multivariate calibration; spectral chemometrics; Eu3+; Dy3+; La2O2S

Acknowledgements

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Ab initio calculations of ABO3 Perovskite (001) Surfaces, Interfaces, and Oxygen Vacancies Therein

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We review the results of B3LYP and B3PW calculations, dealing with ABO perovskite (001) surfaces, heterostructures, and oxygen vacancies therein [1-8]. According to carried out B3LYP and B3PW-simulations, almost all upper layer atoms on the BO_2 and AO-terminated STO, BTO, PTO, CTO, SZO, BZO, PZO, and CZO perovskite (001) surfaces shifts inwards. Practically all ABO perovskite second layer atoms shifts upwards. Finally, nearly all third layer atoms, once more, shifts inwards [1-5]. The ABO perovskite (001) surface energies, for both BO_2 and AO-terminations, are comparable. Computer simulations in the ABO perovskites indicate a significant rise of the B-O chemical bond covalency nearby the BO_2-terminated (001) surfaces in comparison to their bulk. B3LYP and B3PW simulated ABO perovskite bulk G-G band gaps are decreased nearby their BO_2 and AO-terminated (001) surfaces. We discuss recent B3PW-simulations for the STO/BTO, STO/PTO, and SZO/PZO (001) heterostructures [6]. Simulated optical band gaps of the STO/BTO, STO/PTO, and SZO/PZO (001) heterostructures mainly depends on the BO_2 or AO-terminations of the upper layer of the augmented film [6]. The displacement magnitudes of the nearest neighbor atoms, around the (001) surface oxygen vacancy, in the ABO perovskites, usually, are larger than in their bulk [7,8]. In the STO, BTO, PTO, and SZO perovskites, the electronic charge, ordinarily, is a lot better localized interior the bulk than the (001) surface oxygen vacancy [7,8]. In the STO, BTO, PTO, and SZO perovskites, the (001) surface oxygen vacancy induced defect levels are located closer to the conduction band bottom than in the bulk cases. Simulated formation energy difference between the bulk and the (001) surface oxygen vacancies in the STO, BTO, PTO, and SZO perovskites triggers the oxygen vacancy segregation from the bulk towards the (001) surface [7,8].

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Keywords

ABO3 perovskites, (001) surfaces, interfaces, oxygen vacancies

Acknowledgements

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Ionic thermoelectric energy harvesting and storage using nanoconfined aqueous electrolytes

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The growing demand for sustainable energy drives interest in capturing low-grade thermal energy from the environment and industrial processes. Ionic thermoelectric (*i*-TE) materials convert temperature differences into electrical energy via ion thermodiffusion and have gained attention for their potential to generate higher thermopower with aqueous electrolytes. Practical applications face challenges related to stability, energy density, and the integration of energy harvesting with storage. Nanoconfinement presents a promising strategy to address these issues by modifying ion transport, improving ion–solvent interactions, and enhancing charge separation under thermal gradients.

This study explores the thermodiffusion of sodium ions in aqueous electrolytes confined within a nanoporous matrix (anodic alumina, silica or biopolymer-based). Applying a temperature gradient increases the output voltage by boosting charge separation within the nanochannels, where electrical double layers overlap. The unique characteristics of ion transport in these nanochannels were analyzed using electrochemical impedance spectroscopy and cyclic voltammetry. The fabricated *i*-TE system was assembled with intercalation-type electrodes, and its feasibility for energy harvesting and storage has been demonstrated. This work highlights nanoconfinement as an effective approach to improving the efficiency of waste-heat-to-electricity conversion and storage in liquid-electrolyte-based *i*-TE materials.

Keywords

ionic thermoelectrics, nanoconfinement, energy storage, porous silica, waste heat

Acknowledgements

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Versatile Solution-Based Synthesis of Nanostructured Thermoelectric Materials with Their Transport Property Evaluation

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Thermoelectric (TE) materials enable the direct conversion of thermal energy into electrical power and hold considerable promise for sustainable energy technologies. Bismuth and antimony chalcogemnites-based compounds remain the most effective materials near room temperature; however, their broader adoption is limited by expensive synthesis routes, limited scalability, and performance variation across batches. Overcoming these limitations requires synthesis strategies that enable precise control over material quality, morphology, and reproducibility.

In this work, a high-throughput, solution-based chemical synthesis approach is presented for producing nanostructured Bi_2Te_3 using microwave-assisted heating. This method provides energy-efficient volumetric heating that supports rapid reaction kinetics, high product yields, and excellent reproducibility. Several bottom-up solution synthesis techniques, including hydrothermal, polyol, and thermolysis routes, are employed to systematically examine the effects of the solvent environment and precursor chemistry on particle morphology, crystallinity, and surface characteristics.(*1–3*)

The resulting n-type nanostructured Bi_2Te_3 materials are systematically characterized regarding their structural, morphological, and TE transport properties. The findings show that solution synthesis provides effective control over nanostructure formation, morphology, and surface chemistry while maintaining the materials' phase purity and performance, highlighting its potential as a versatile and scalable method for synthesizing metal chalcogenide-based TE materials.

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Keywords

Thermoelectrics, Solution Synthesis, Nanostructuring, Energy Harvesting.

Acknowledgements

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How stable are mixed-metal chalcohalides?

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Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs with sum formula: $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaics[1,2], capable of delivering high conversion efficiencies[3]. Yet, their thermodynamic stability remains largely unexplored.

We assess the thermodynamic stability of 54 MMCH compounds by modelling their phase diagrams using DFT, *pymatgen* tools from the Materials Project[4] and the Alexandria Materials Database[5]. Figure 1 a) illustrates, for example, the 4D phase diagram of $Sn_2InS_2Br_3$. All studied MMCHs lie above the convex hull, independent of their space group (*Cmcm*, $Cmc2_1$, $P2_1/c$). Accounting for computational uncertainty (mostly from the applied exchange-correlation functional) moves a considerable fraction of MMCHs close to or below the hull. The MMCH decomposition paths follow five reactions, with 4 $M(II)_2M(III)Ch_2X_3$ -> 2 $M(III)_2Ch_3$ + 6 $M(II)X_2$ + 2 M(II)Ch occurring most frequently. Figure 1 b) presents a 2D projection of the convex hull surface (cyan) containing $Sn_2InS_2Br_3$. The vertices of the hull surface correspond to the thermodynamically stable decomposition products. Experiments from collaborators show that compounds close to the convex hull can be synthesized, whereas compounds far from the hull decompose following the predicted reactions. Overall, our results show that MMCHs are synthesizable, but fabrication conditions need further optimisation.

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Keywords

mixed-metal chalcohalides, phase diagrams, thermodynamic stability, decomposition reactions, density functional theory

Acknowledgements

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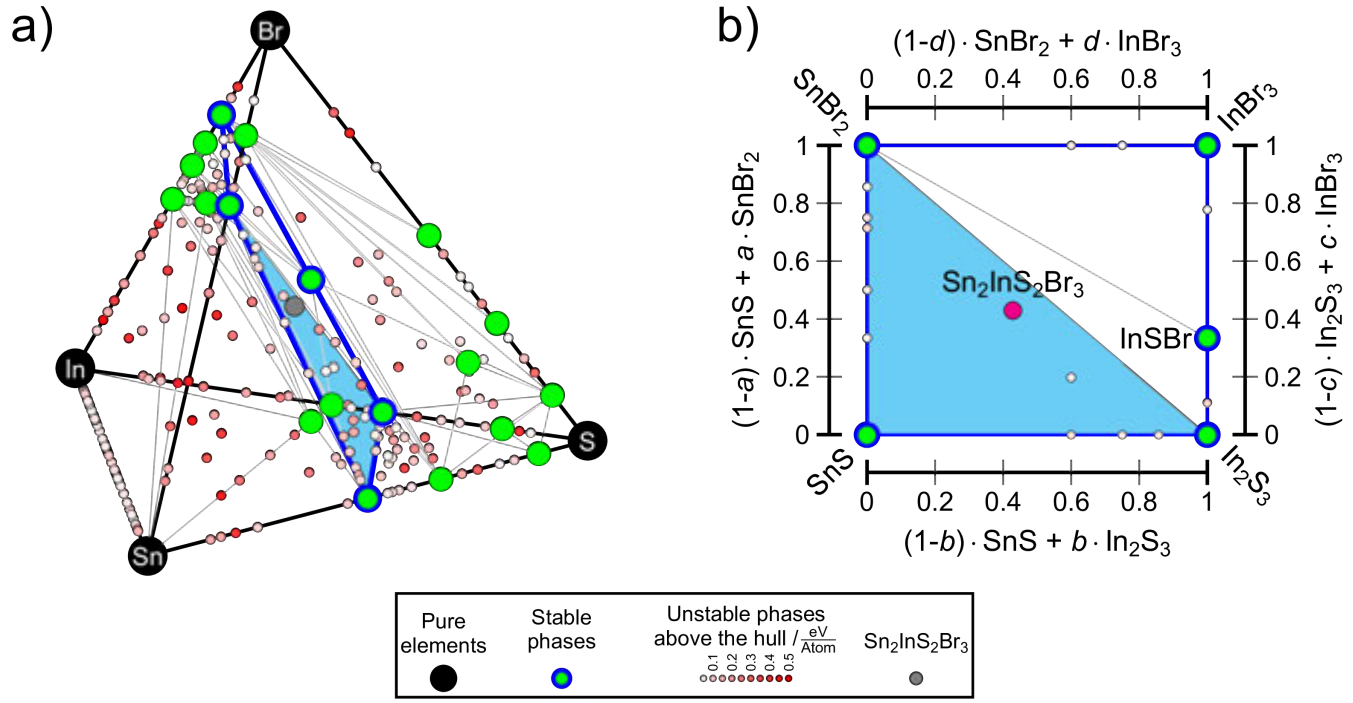


Induced piezoelectric effect in cubic materials and improvement of the temporal response

Reinis Ignatans , Institute of Solid State Physics - University of Latvia

Reinis Ignatans , Institute of Solid State Physics

Discovery of the giant induced piezoelectric effect in gadolinium doped cerium oxide has fuelled the search for unconventional electromechanically active materials. Although, piezoelectricity in ceria and other related cubic materials is formally forbidden by the centrosymmetric nature of the unit cell, the symmetry can be broken by the interplay of the defects within the material and the DC electric field.

Here induced piezoelectric effect is demonstrated in $Hf_{0.5}Zr_{0.5}O_2$ thin films, with particular emphasis on the *in situ* electric field X-ray diffraction measurements, which reveal extrinsic nature of the induced electric field strain in particular material if compared to macroscopic interferometric strain measurements. $Hf_{0.5}Zr_{0.5}O_2$ also shows new way of breaking inversion symmetry via electrostriction driven strain.

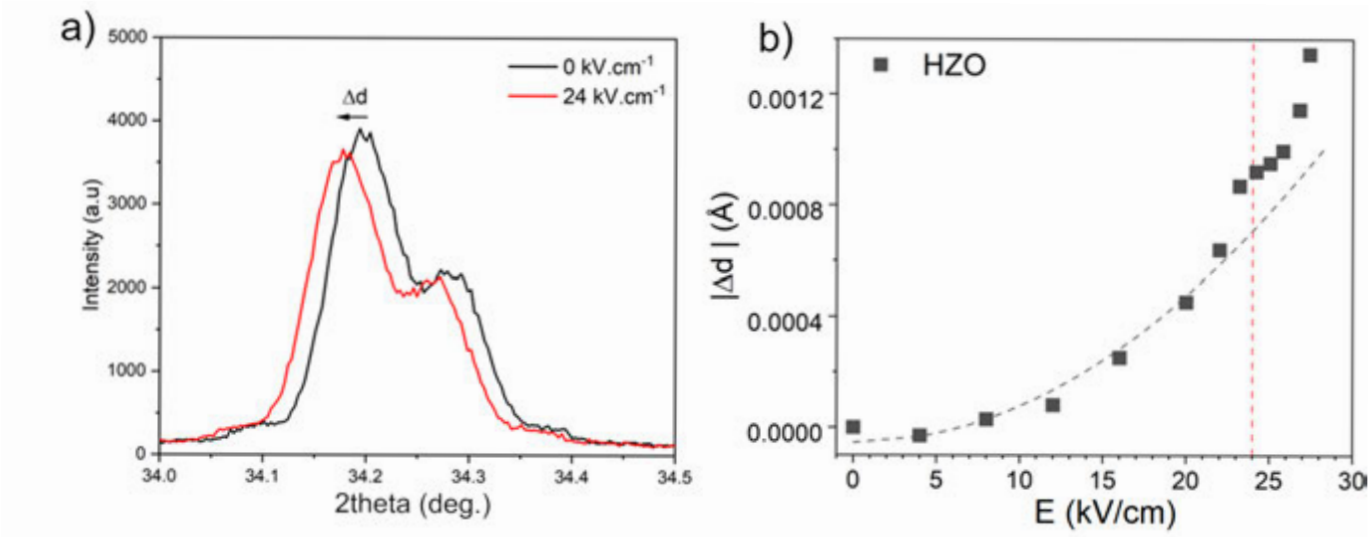
At the moment giant induced piezoelectric effect in $Hf_{0.5}Zr_{0.5}O_2$ or CeO_2:Gd is large only at comparably low driving field frequencies (i.e. below 1 kHz), which is one of the main drawbacks of such materials for practical implementation. Therefore, here a combined thin film device is proposed consisting of CeO_2:Gd and traditional piezoelectric $BaTiO_3$ layers with the idea of improving high frequency electromechanical response. The devices are studied with *in situ* electric field XRD and laser interferometric methods.

Keywords

Piezoelectricity, in situ XRD, symmetry breaking

Acknowledgements

Reinis Ignatans acknowledges financial support from Latvian Council of Science under the grant: "New generation of piezoelectric materials for active vibration control" (grant no. LZP-2023/1-0571).


a)
0 kV.cm-1
24 kV.cm-1
Δd
Intensity (a.u)
2theta (deg.)
b)
HZO
|Δd | (Å)
E (kV/cm)

Atomic Drums Without Order

Liga Jasulaneca , Institute of Solid State Physics, University of Latvia

Atomically thin suspended membranes provide a powerful platform for studying mechanical motion at the ultimate limits of mass and thickness. To date, most atomic-scale nanomechanical resonators have relied on crystalline two-dimensional materials, where long-range lattice order governs mechanical behavior. In contrast, the vibrational properties of amorphous materials in the two-dimensional limit remain largely unexplored.

Here we demonstrate nanomechanical resonators fabricated from freestanding monolayer amorphous carbon (MAC) [1], a structurally disordered yet mechanically robust two-dimensional material. Using photothermal actuation and interferometric readout [2], we resolve thermally driven Brownian motion and characterize the driven response across linear and nonlinear regimes. The devices exhibit pronounced nonlinear dynamics, including nonlinear stiffness and damping, as well as parametric modes under direct excitation.

Our results provide first experimental access to a wide range of dynamic phenomena in amorphous monolayers, positioning MAC as a viable platform for two-dimensional nanomechanical resonators. The robustness of MAC membranes make them attractive for sensing applications, including nanomechanical detection of bacterial motion and other biological activity.

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Keywords

nanomechanical resonators, monolayer amorphous carbon, nanosensors, nonlinear nanomechanics, nanomotion

Materials for Energy

Supercapacitors: Principles and Electrochemical Measurement Techniques

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Supercapacitors are commonly evaluated using electrochemical techniques such as cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. Each method provides different information about the charge-storage behavior of an electrode or device, including capacitance, internal resistance, rate capability, reversibility, stability, and ion-transport limitations. However, reported performance values strongly depend on measurement configuration, voltage window, current density or scan rate, electrode mass loading, and capacitance calculation method. Therefore, careful reporting and interpretation of experimental conditions are essential for meaningful comparison between materials and devices.

This talk provides an overview of how these measurement techniques are used, what information can be extracted from them, and what common mistakes should be avoided during data interpretation.

Keywords

Supercapacitor, electrochemical analysis, GCD, CV, EIS

Acknowledgements

This work was supported by the European Commission's Horizon Europe programme through the project Atomic Layer-coated Graphene Electrode-based Micro-flexible and Structural Supercapacitors, grant agreement ID 101120677. The project forms part of the Graphene Flagship initiative, which supports the development of graphene and other two-dimensional material technologies.

Self-Assembled 2D Peptide Crystals and Thin Films

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Bioinspired supramolecular peptide-based materials are emerging as promising building blocks for bioelectronic devices, including energy harvesting and energy storage systems [1,2]. These materials attract considerable interest due to their biocompatibility, environmental friendliness, chemical diversity, and ability to self-assemble into hierarchical nanostructures with unique physical properties. Among peptide nanostructures, two-dimensional (2D) crystals and thin films are particularly attractive for practical applications, although they remain relatively underexplored [3,4].

Piezoelectricity in 2D materials has gained increasing attention because it enables the development of thin, lightweight, and flexible devices. Unlike conventional three-dimensional piezoelectric materials, whose properties often degrade at reduced dimensions, piezoelectricity in 2D systems can be enhanced by surface and flexoelectric effects. However, most known 2D piezoelectric materials exhibit mainly in-plane responses, typically requiring mechanical bending of flexible substrates for device operation. As a result, understanding out-of-plane piezoelectricity in such materials remains an important challenge.

In this work, we synthesized crystalline structures based on several dipeptides—diphenylalanine (FF), dileucine (LL), phenylalanine–glutamic acid (FE), and tryptophan–glycine (WG)—using solid-phase crystallization. These dipeptides self-assemble into layered crystals composed of two-dimensional sheets held together by weak non-covalent interactions and forming thin films. The resulting structures exhibit high crystallinity and a pronounced piezoelectric response, highlighting their potential for energy harvesting and storage applications.

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Keywords

piezoelectricity, peptide film, energy harvesting

Acknowledgements

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Accelerating Atomic Configuration Identification on Reconstructed Surfaces with Machine Learning

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Surfaces of solid state materials play a crucial role in many technological applications, such as heterogeneous catalysis connected with production of green fuels or preparation of semiconductor devices. However, the atomic surface structure of many materials are still unknown, even in the most simple case of surfaces in vacuum, leaving a huge knowledge gap of physics and chemistry of surfaces. In the past the computational search for the atomic structure of surfaces has been driven by chemical intuition or ab-initio molecular dynamics. But the recent developments in machine learning (ML) allows for going beyond the limits of computational approaches.

In this work, I am presenting my ML aided workflow for predicting the atomic structure of surfaces, mainly for semiconductors and oxides: Starting from automatized tool for passivation of bottom side to reinforcement learning based tool able to build few top layers of (reconstructed) surface, enhancing the original strategy by [1]. To speed-up and computationally cheapen the workflow, I will be employing already pre-trained ML interatomic potentials, like MACE-MP [2]. Simultaneously, I will be complementing to development of the pre-trained (universal) potential to be better working on a surfaces.

Through this tool, I aim to seal the knowledge gap and therefore contribute to development of new semiconductor devices or heterogeneous catalysts for cheaper production of green fuels.

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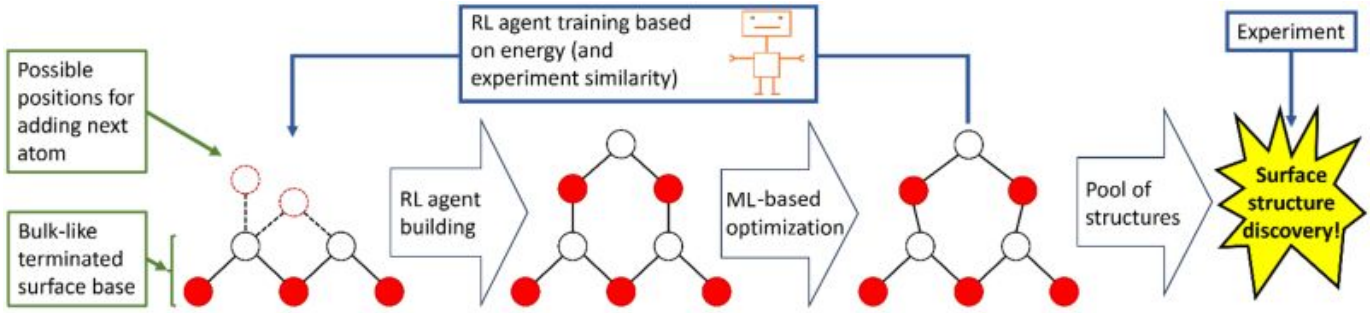
Keywords

Machine-learning, Surface Science, Machine-learned interatomic potential



Study of thin Py films suitable for excitation of surface spin-wave

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Tetiana Kalmykova , Institute of Electrical Engineering SAS, Department of radiospectroscopy O. Ya. Usikov Institute for Radiophysics and Electronics NAS of Ukraine

This study examines how deposition parameters influence the magnetic properties of thin permalloy (Py, $Ni_{80}Fe_{20}$) films fabricated via electron-beam evaporation using an AJA Orion 8E system. The objective is to produce uniform Py films with a ferromagnetic resonance (FMR) linewidth of 15–20 Oe in the 5–6 GHz range—an essential specification for applications in microwave technologies and spintronic devices [1], [2]. These films are particularly suited for exciting and amplifying surface spin waves in planar microwave antennas incorporating Inverse Split Ring Resonators (ISRRs)[3].

We conducted a comparative study on different substrate types, including sapphire and silicon substrates with varying SiO layer thicknesses, to assess their effect on magnetic performance. Deposition temperature was also varied: moderate heating to 200 °C led to slight improvements in FMR linewidth, whereas higher temperatures (400 °C) degraded magnetic quality.

The influence of stray magnetic fields within the deposition chamber was explored by shielding the samples with a metallic ring, though this showed no measurable improvement. To address this, ongoing experiments are investigating deposition under a constant 40 mT out-of-plane magnetic field. Additionally, the effect of sample rotation during deposition on FMR linewidth is currently under investigation.

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Keywords

ferromagnetic resonance, spin-wave, spintronics.

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FIRST PRINCIPLES STUDIES OF TERNARY HEXAFLUORIDES AS SCINTILLATORS FOR MEDICAL IMAGING TECHNOLOGIES

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Marco Kirm , Institute of Physics, University of Tartu, Estonia
Juhan Matthias Kahk , Institute of Physics, University of Tartu, Estonia

Scintillators are materials that convert ionizing radiation into detectable low-energy radiation and are crucial in applications such as medical imaging technologies like computed tomography (CT) and positron emission tomography (PET) [1]. In time-of-flight PET (TOF-PET), the signal-to-noise ratio and spatial resolution are directly related to the coincidence time resolution of scintillator detectors [2]. The discovery of new scintillators with higher yield and shorter response times would enable the development of more efficient and accurate detectors, potentially allowing for higher-resolution images and reduced radiation doses to patients. However, experimental testing of scintillator materials is time-consuming and requires expensive specialized equipment, making computational identification of promising candidates highly desirable [3].

In this work, we investigate one of the inorganic ternary hexafluorides—K_2SiF_6, using first-principles methods. Initial Density Functional Theory (DFT) calculations were used to analyze their electronic structures, and results were compared to experimental measurements from optical absorption, luminescence, and photoemission spectroscopy.

Building on this, we employed many-body perturbation theory within the GW approximation using the BerkeleyGW code to compute quasiparticle energy levels of K_2SiF_6. The GW calculations significantly increase the predicted band gap compared to DFT and provide a more reliable description of quasiparticle electronic structure. These results offer improved insight into the electronic properties of K_2SiF_6 and its potential suitability as a scintillator material.

Future work will extend these advanced calculations to the other compounds in the series and incorporate excitonic effects via the Bethe-Salpeter Equation, along with the investigation of phonon-assisted processes in the optical response.

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Keywords

Scintillators, First Principle Inestigation, Electronic Structure, Photoelectron Spectrum, BerkelyGW

Acknowledgements

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Comparative Analysis of Nanostructures Formation in Semiconductors by Laser Irradiation and Stranski-Krastanov Methods.

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Nanostructures (NSs) are the most investigated objects in solid-state physics, especially the Quantum confinement effect (QCE) in quantum dots – 0D, quantum wires - 1D, and quantum wells – 2D systems. Because under these conditions, a change in the band structure of a semiconductor takes place. This leads to a crucial change in the physical properties of a semiconductor, and new possibilities for constructing electronic and optical devices are demonstrated [1]. Today, for NSs formation, very often molecular beam epitaxy [2], ion implantation [3], chemical vapor deposition [4], sol-gel [5], spray pyrolysis [6], magnetron sputtering [7], and laser ablation [8] with the following thermal annealing Stranski-Krastanow method [9] are used. Using these methods, NSs mostly grow randomly. It impedes the development of nanotechnology.

Twenty years ago, we found a new quantum system, the so-called Quantum cone on the surface of a Ge crystal after irradiation by Nd:YAG laser [10]. Late in Si [11], GaAs, CdZnTe single crystals, and SiGe solid solution, which possesses unique optical properties: a huge “blue shift” of photoluminescence (PL) spectrum, high intensity of PL, and “redshift” of LO phonon line frequency in Raman spectrum. Irradiation of Si crystal by Nd:YAG laser has led to the formation of nano cones which possess a unique PL spectrum: “blue shift” on 1.1 eV, an asymmetric, wide PL band of rainbow-like spectrum. Moreover, metallic Zn nanostructures arise on ZnO crystal after irradiation by the laser [12]. Advantages of the Laser irradiation method, compared to the Stranski-Krastanow method, include the ability to control the position and height of the cones via laser intensity and dose, and the use of homojunctions, which expands the range of materials and structures for forming nanostructures. Moreover, the laser irradiation method has a low economic cost: no need for a vacuum or special gas, and a short process time.

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Keywords

Laser, Stranski-Krastanov, Ge, Si, GaAs, CdZnTe, SiGe, ZnO, Raman, photoluminescence

Compute-Me-(Not): The bulky groups attached to nonlinear optical chromophores

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Kirils Dmitrijevs , Riga Technical University
Kaspars Traskovskis , Riga Technical University
Mārtiņš Rutkis , Institute of Solid State Physics, University of Latvia

Nonlinear optical materials enjoy applications in electro-optical modulators and other photonic devices [1]. The second-order nonlinear optical active materials typically consist of either non-centrosymmetric monocrystals or of organic chromophores mixed into polymeric films and oriented under the applied voltage [2]. The ordered state thus achieved is gradually lost in time, which is typically mitigated by attaching bulky groups to chromophore-containing molecules [3].

Computational assessment typically precedes the experimental characterization of materials. However, bulky groups are a snag. The usual strategy (excluding them from the model) decreases the computation time and apparently doesn't introduce any significant perturbations. The latter hunch doesn't abide in truth, however. First, orientation of these groups directly changes the dipole moment. Second, the centrifugal forces from the reorientation of bulky groups can substantially deform the π-electron-conjugated backbone and thus change the value of the nonlinear optical activity descriptor β.

This problem can be addressed, e.g., by molecular dynamics. However, this isn't easily applied to extended π conjugation. The present study considers another approach: to obtain the geometries of terminal cases of bulky group positions with respect to the π electron system and to each other. We can thus provide the margins within which β could possibly lie for the correlation with experimental data.

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Keywords

first hyperpolarizability, nonlinear optics, quantum chemistry, bulky groups, aggregation, functional materials

Acknowledgements

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Quantum Magnetometry in the University of Latvia: Towards Functional Prototypes

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Building on extensive fundamental research in light-matter interactions, the Laser Centre at the University of Latvia has transitioned toward the development of quantum sensors. By exploiting quantum mechanical processes sensitive to external electric and magnetic fields, these devices can achieve unprecedented sensitivity levels beyond the classical limits. This presentation details the methods for sensing and some functional prototypes across two primary sensing media: (i) defects in diamond (Nitrogen-Vacancy (NV) centers) and alkali-metal atomic vapors. We present key results from recent and ongoing projects, highlighting the steps towards the transition from laboratory and theory to hardware development. We further discuss the integration of these sensors into different application areas, including high-resolution magnetic field imaging, geomagnetic mapping for navigation, and non-invasive biomagnetic sensing.

Keywords

quantum sensors; atomic; NV in diamond; magnetic field;

Acknowledgements

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Investigation of crystal structures, stability, electronic structure and optical properties of XH3-2xOx (X=Y, La, Nd, Nb, Zr) oxyhydrides by first–principles calculations

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Mixed–anion oxyhydrides are a versatile class of materials combining structural diversity with tunable electronic and optical properties. We investigate multication oxyhydrides $XH_{3-2x}O_x$ (X=Y, La, Nd, Nb, Zr) using density functional theory within VASP. The selected cations provide complementary roles: Y as a photochromic host, La and Nd as large–radius lattice softeners, Nb contributing d–electron states, and Zr enhancing structural stability. Such combinations are expected to enable structural motifs inaccessible in single–cation systems and are relevant for high–entropy compositions.

Crystal structure prediction was performed with evaluation of total energies, dynamical stability, and anion–cation geometric compatibility. Several stable and metastable fluorite–like and distorted fluorite–derived configurations were identified. Lattice parameters follow trends expected from averaged ionic radii and mixed H^-/O^{2-}sublattice geometry.

Electronic structure analysis (DOS, band structures, charge density) reveals semiconducting behavior with band gaps strongly influenced by cation size mismatch and local strain. Optical properties, obtained from frequency–dependent dielectric functions and absorption spectra, show tunable near–edge response governed by mixed–anion chemistry and cation–driven band modifications. Bonding analysis indicates coexistence of ionic and covalent interactions, underpinning structural flexibility and functional tunability.

Keywords

mixed-anion oxyhydrides, high-entropy multication systems, density functional theory (DFT), crystal structure prediction, electronic and optical properties

Acknowledgements

The work has been funded by the Latvian Council of Science Project through the No. lzp-2024/1-0632. Norwegian NOTUR supercomputing facilities have been used in the computations through the project nn4608k.

Influence of europium ion doping on photoinduced properties of 2D cobalt hydroxide

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The persistence of emerging pollutants such as pesticides and antibiotics in wastewater highlights the need for low-energy treatment technologies.[1,2] Transition-metal hydroxides are considered good matrices for photocatalysis due to their abundance, low cost, and favourable electronic structures.[3-5] In particular, the properties of cobalt hydroxide, an emerging electro- and photocatalyst, can be tuned through rare-earth doping, which increases the light absorbance and charge transfer at the surface, a crucial factor in any photocatalytic applications.

We report the hydrothermal synthesis of europium-doped cobalt hydroxide nanoplates ($Co(OH)_2$:Eu, 2.8 wt%) and evaluate their structural, electronic, and functional properties relative to undoped $Co(OH)_2$.[6] Europium incorporation improves the stability of the material compared to the undoped hydroxide. Photocatalytic performance was assessed via methylene blue degradation, supported by band-structure analysis and radical-scavenger studies to elucidate the reactive pathways.

We established that $Co(OH)_2$:Eu possesses the local state above the conduction band edge, which induced a marked increase in the negative photoconductivity of $Co(OH)_2$:Eu due to the binding of electrons, highlighting the potential use of rare-earth doping in optoelectronic switches. The enhanced activity of $Co(OH)_2$:Eu demonstrates the effectiveness of rare-earth doping in tailoring transition-metal hydroxides for pollutant degradation and multifunctional photoactive applications.

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Keywords

photocatalysis, negative photoconductivity, cobalt hydroxide, rare-earth doping

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Plasmonic Silver Nanoparticles: Synthesis and Optical Response

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Aivars Vembris , Institute of Solid State Physics, Latvia
Christophe Couteau , University of Technology of Troyes, France

ic Controlled synthesis of plasmonic silver nanoparticles (AgNPs) provides precise adjustments of they optical properties for advanced photonic and plasmonic application. Plasmonics is the study of how light interacts with free electrons in metals at the nanoscale, producing surface plasmons that strongly concentrate electromagnetic fields near the particle. AgNPs were produced via chemical route with well-defined morphology and characterizes using SEM. UV–Vis spectroscopy showed distinct surface plasmon resonance peaks whose positions correlate with particle size and shape, demonstrating how plasmonic behavior can be engineered for photonic device integration. These findings highlight the potential of plasmonic nanostructures for enhanced optical sensing and nanoscale light manipulation.

Keywords

Nanoparticle synthesis, nanomaterials, plasmonic, emission.

Acknowledgements

This work was carried out within the ToEQPL project, which received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101160101.

Technical Parameters and Principles of Charging and Discharging in Lithium-Ion Batteries

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Gints Kucinskis , Institute of Solid State Physics University of Latvia

Ni-rich layered cathodes like NCM811 are key to next-generation lithium-ion batteries (LIBs) thanks to their high capacity. However, polarization and structural degradation at high voltages severely limit performance. Grasping how voltage windows, charge/discharge rates, and impedance changes interact is vital for boosting cycle life and energy efficiency.

We conducted electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), direct current internal resistance (DCIR) measurements, and extended cycling tests on NCM811 cells. Tests varied cut-off voltages (3.8–4.25 V) and C-rates (0.2C–1C). Equivalent circuit models helped derive charge transfer resistance (Rct*Rct*) and diffusion parameters.

Nyquist plots showed minimal Rct*Rct* around 3.8 V, with a steep rise above 4.1 V—linked to CV-detected phase transitions. Cycling results indicated optimal capacity retention at moderate C-rates.

Maintaining an upper cutoff ≤ 4.3 V and avoiding extreme cycling rates ensures a favorable balance between energy efficiency and structural stability, significantly extending cell lifetime. These results provide practical guidelines for battery management system (BMS) voltage cutoffs and charging protocols for next-generation LIBs.

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Keywords

Li batteries, NCM811, EIS

Acknowledgements

This work was supported by the Horizon Europe project “Eliminating VOC from Battery Manufacturing through Dry or Wet Processing” (NoVOC), Grant Agreement No. 101069612.

Towards high-volume scale-up of ALD coatings for battery and supercapacitor applications

Tero Pilvi , Beneq oy

Andrew Cook , Beneq Oy

Atomic layer deposition (ALD) is an advanced coating technique, which has been studied for more than 10 years for uses in battery and supercapacitor applications on small scale batch systems. ALD technology has been shown to improve battery and supercapacitor performance, through the introduction of thin film coatings to modify interface surfaces on cathode and anodes. This presentation will demonstrate how Beneq uses R2R ALD and large batch systems to scale production levels for high-throughput manufacturing.

Keywords

ALD, R2R, supercapacitor, battery

Comparative Study of Thermal, Current-Induced, and Laser-Induced Melting of Ag and Au Nanoplates

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Understanding melting mechanisms in low-dimensional metallic nanostructures is essential for their reliable integration into nanoelectronic, plasmonic, and sensing applications. In this work, we present an ongoing experimental study of melting behavior in silver (Ag) and gold (Au) nanoplates under three distinct excitation modes: (i) uniform thermal heating, (ii) current-induced (Joule) heating, and (iii) laser-induced plasmonic heating.

Experiments are performed inside a scanning electron microscope (SEM) equipped with a heating stage, enabling in situ observation of thermally driven morphological transformations. Localized Joule heating is achieved using nanomanipulators inside the SEM chamber, allowing controlled current injection through individual nanoplates. Plasmon-assisted melting is investigated using a 532 nm pulsed green laser delivered via an optical fiber, enabling localized excitation and non-equilibrium heating.

By directly comparing these three melting pathways within the same experimental platform, we aim to distinguish differences in melting thresholds, morphological evolution, and resolidification behavior. Special attention is given to size-dependent effects, surface diffusion, edge rounding, Rayleigh-type instabilities, and substrate interactions.

This study is currently in progress. Preliminary observations indicate distinct transformation kinetics and morphology evolution depending on the excitation mechanism, suggesting fundamentally different energy deposition pathways and thermal gradients at the nanoscale.

The results will contribute to a deeper understanding of nanoscale phase transitions under equilibrium and non-equilibrium conditions and provide insight into the stability limits of plasmonic and nanoelectronic metallic components.

Keywords

Ag and Au nanoplates, in-situ SEM experiments, plasmonic melting, nanomanipulations

Acknowledgements

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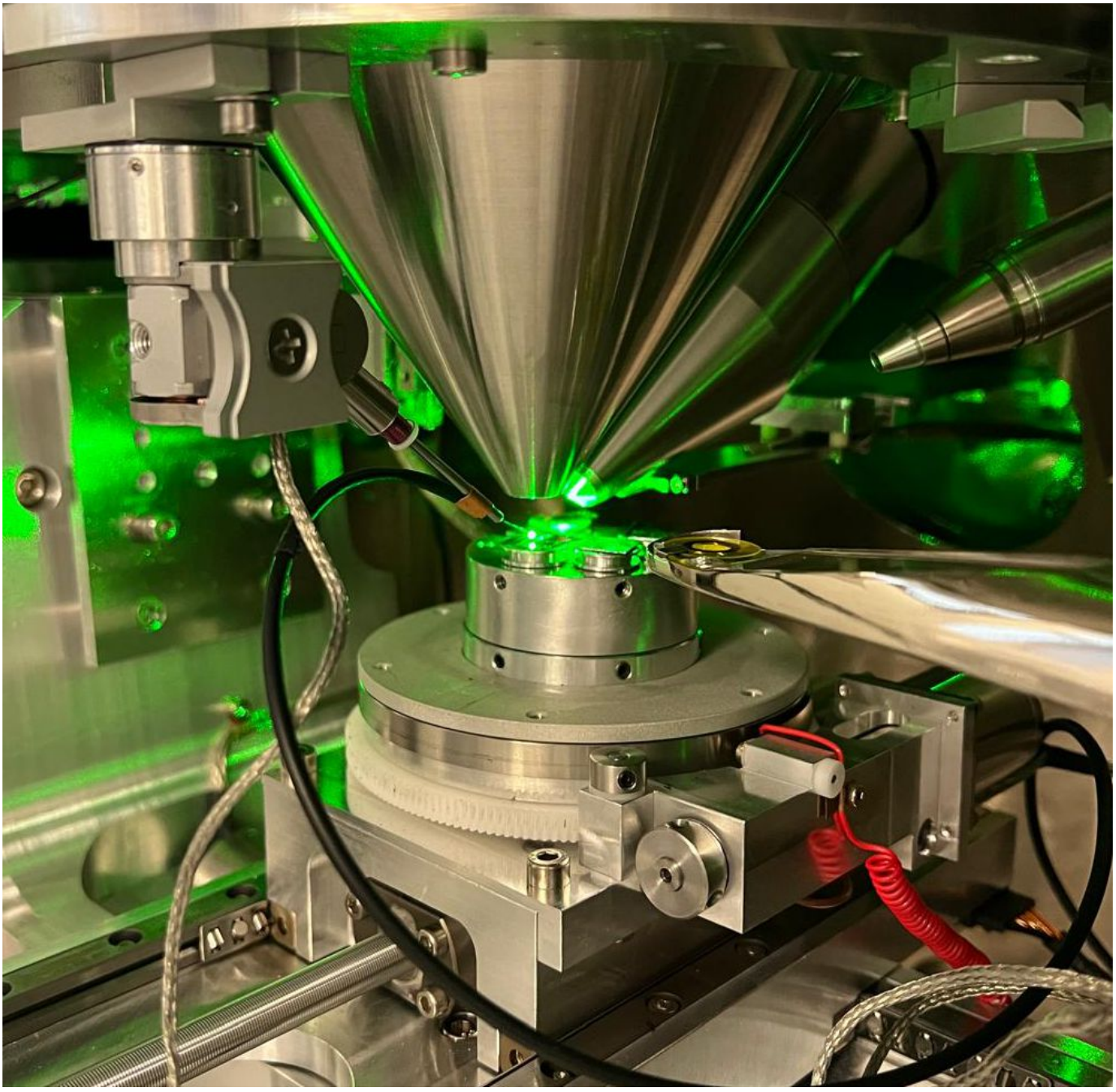

Sustainable Graphene-Based Supercapacitors: From Advanced Materials to Scalable Device Integration

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The ARMS project is developing a sustainable and scalable approach to next-generation supercapacitors by combining advanced graphene-based materials, bio-derived carbons, and environmentally friendly processing routes. The goal is to achieve energy densities above 50 Wh/kg while maintaining high power performance, long cycle life, and compatibility with industrial-scale manufacturing.

Recent progress has been strong across all development areas. High-surface-area bio-based activated carbons have been successfully optimized, reaching up to 2844 m^2/g surface area and 265 F/g capacitance, and are now being integrated into scalable electrode formats. Graphene-enhanced electrodes have shown further performance gains, with specific capacitance values reaching ~307 F/g, excellent conductivity, and clear pathways toward roll-to-roll and printing-based production.

On the materials engineering side, ultra-thin atomic layer deposition coatings (such as TiO_2 and MnOx) have been introduced to porous electrodes, improving capacitance by up to around two times while maintaining pore accessibility. In parallel, new hybrid electrolyte systems have been developed that improve safety and stability, enabling operation up to 2.3 V and supporting flexible and structural device concepts.

Early-stage device integration has begun, including pouch cell fabrication and structural laminate prototypes, demonstrating the feasibility of translating material-level improvements into practical energy storage devices. Alongside this, sustainability-by-design assessments are being used to guide material selection and identify environmental hotspots early in the development cycle.

Overall, the project is moving steadily from advanced materials toward integrated, manufacturable supercapacitor devices with improved energy density, safety, and sustainability.

Keywords

Graphene supercapacitors; Sustainable energy storage; Bio-based activated carbon; Atomic layer coatings; Hybrid electrolyte systems

Acknowledgements

This project, funded by the European Commission's Horizon Europe programme, is part of the Graphene Flagship initiative which works to advance technologies that rely on graphene and other 2D materials.

Luminescence properties of Cs2HfF6: the observation of self-trapped and perturbed excitons using synchrotron radiation

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Heavy ternary compounds with high stopping power are attractive for potential applications in radiation detection technologies. Extensive studies of some representatives of the Cs_2HfX_6 (X = I, Br, Cl) family with a vacancy-ordered double perovskite structure have shown that the origin of their bright scintillation is due to emission from self-trapped excitons[1,2]. Only defect related emission has been studied in the wide-gap ternary fluoride Cs_2HfF_6 up to now[3,4]. We report here on the discovery of exceptionally bright ultraviolet emission of self-trapped excitons and a series of emission bands presumably related to defect-perturbed excitons[5,6] in Cs_2HfF_6 powders and single crystals with a trigonal crystal structure confirmed by XRD (Fig. 1a). Time-resolved cathodoluminescence study revealed the triplet nature of the involved excitons, with long decay times. Luminescence, excitation, and reflectivity spectra were studied for the excitation photon energy range of 4.5 to 45 eV at the FinEstBeAMS beamline of MAX IV laboratory[7]. The reflectivity spectrum (Fig. 1b) of the single crystal showed sharp features corresponding to the high-density 5d Hf, 2p F, and 5p Cs electronic states, which could be directly correlated with electronic band structure calculations[8] by introducing a scissor factor of 3.1 eV (Fig. 1c). Thus, we estimated the real bandgap of Cs_2HfF_6 to ~10.3 eV. These findings will be useful for the future potential applications of the heavy bright UV emitter studied.

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Keywords

Cs2HfF6, Excitons, Synchrotron radiation, Reflectivity, and Band structure

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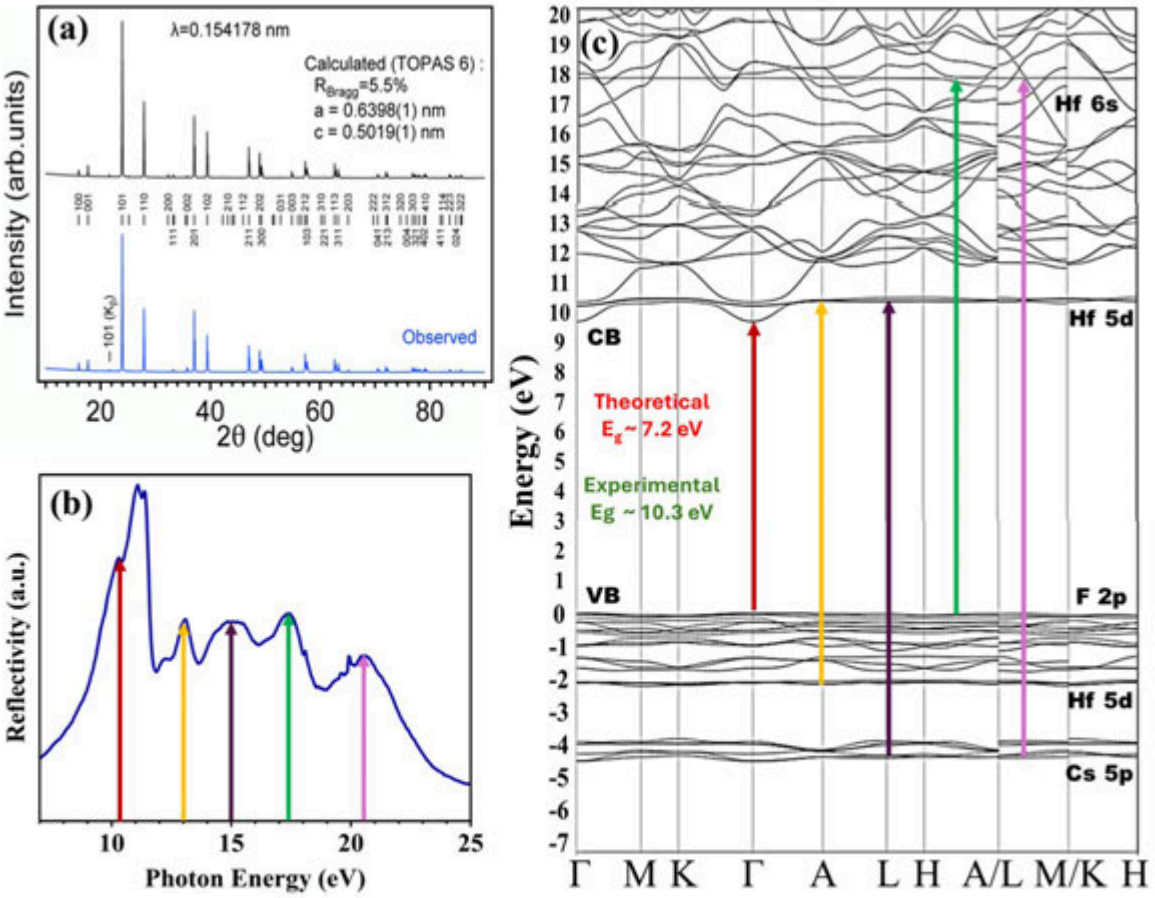

Figure 1. XRD pattern of Cs_2HfF_6 indexed in the trigonal crystal system (a), correlation between the reflectivity (b) and the band structure (c) of Cs_2HfF_6 (The arrow colors in the reflectivity spectrum indicate the corresponding transitions in the band structure).

Ferrite Based Functional Nanomaterials for Practical Applications

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Magnetic nanoparticles have received considerable attention due to their size-dependent physicochemical and magnetic properties, which make them highly attractive for a wide range of applications [1]. Ferrites typically possess a spinel structure, in which metal cations are distributed between tetrahedral and octahedral lattice sites, and even minor variations in cation distribution can significantly affect key properties, including magnetic anisotropy, saturation magnetization, coercivity, and electron-transfer characteristics [2]. This structural flexibility enables the rational design of ferrite materials with application-specific performance, particularly in catalysis, environmental remediation, sensing, biomedicine, and energy-related systems [3]. Compared with many metallic magnetic nanoparticles, ferrite nanoparticles generally exhibit superior chemical stability, enhanced resistance to oxidation, and lower susceptibility to corrosion, making them especially attractive for use in aqueous and oxidative environments.

In this work, ferrite nanoparticles synthesized by the hydrothermal co-precipitation method were characterized, and their specific properties were tuned by modification of surface chemistry. Methods such as TEM, XRD, FTIR, and Raman spectroscopy were employed to analyze materials and to link synthesis parameters to specific ferrite nanoparticle properties.

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Keywords

Ferrite; Nanoparticles; Wastewater Treatment; Environment Remediation; Biomedicine

Acknowledgements

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Lattice Dynamic - Based Design of Light Ion Conductors

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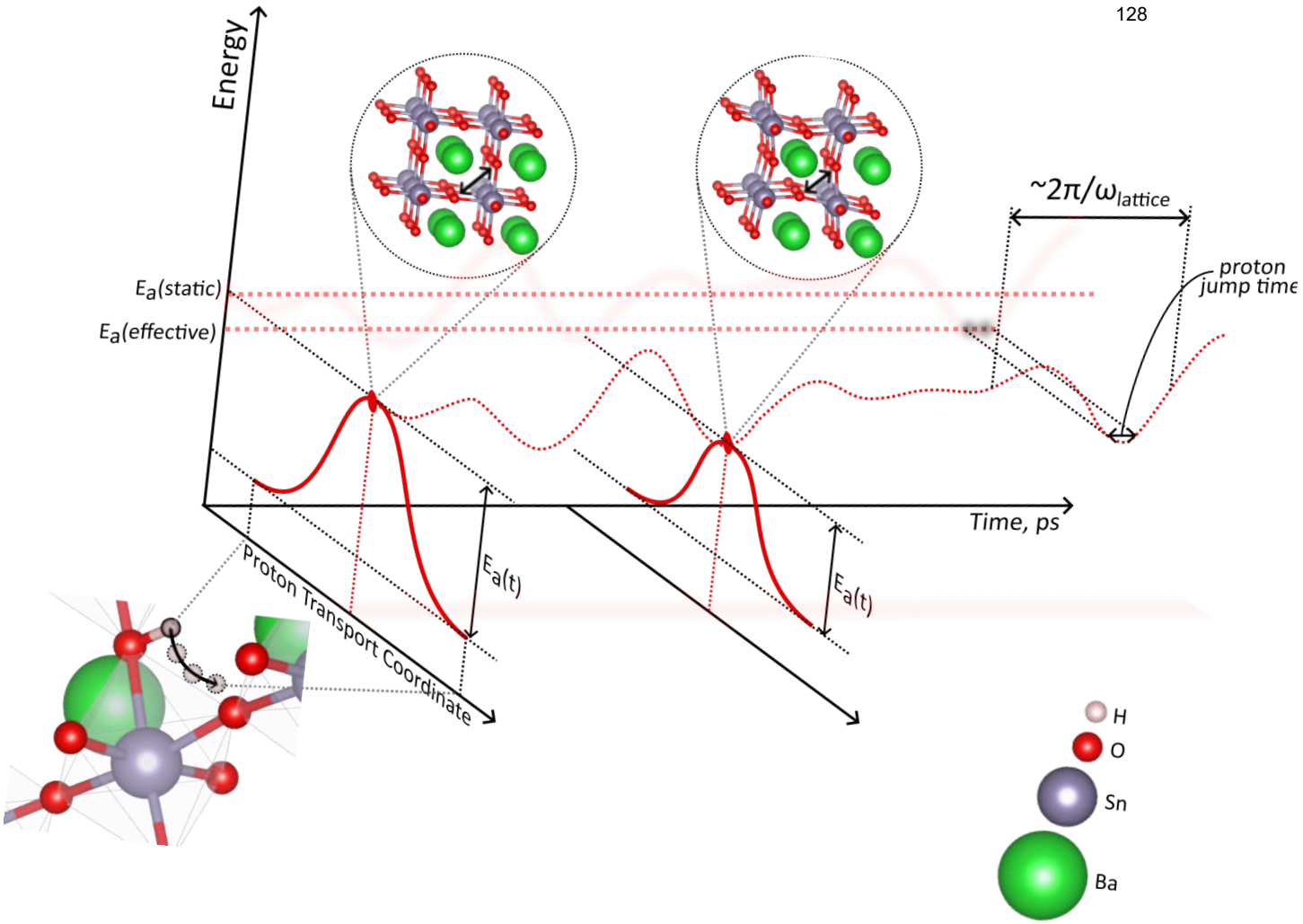
Solid-state ion transport underpins electrochemical energy conversion and storage (fuel cells, Li batteries). Yet *ab initio* barriers for proton hopping in oxide proton conductors often disagree with experimentally measured activation energies and are frequently “corrected” by semi-analytical terms such as dopant–proton Coulomb trapping. We show that the mismatch originates from the migration dynamics of light ions on a peculiar potential-energy surface: the proton can respond much faster than the host lattice, so the lattice cannot fully relax during a jump attempt. Proton motion therefore occurs in a time-dependent energy landscape set by thermal lattice vibrations. Certain vibrational modes periodically drive the local structure toward the transition-state geometry, transiently lowering the barrier; this strongly anharmonic regime is not captured by standard transition-state theory.

We propose a phonon-based framework that separates fast ion motion from slower lattice dynamics and yields an effective migration barrier that includes anharmonic vibrational effects. In this approach, lattice dynamics become a descriptor for ion mobility. We introduce an algorithm that identifies the modes with the strongest barrier modulation, enabling a design principle: softening these modes increases their amplitude and can reduce the effective activation energy. We demonstrate the method for perovskite proton conductors and discuss its applicability to lithium-ion conductors.

Keywords

Proton conductors, Lithium ion conductors, lithium batteries, fuel cells, solid state ionics


Energy
E_a(static)
E_a(effective)
~2π/ω$_{lattice}$
proton jump time
Time, ps
Proton Transport Coordinate
E_a(t)
E_a(t)
H
O
Sn
Ba

Bayesian optimization machine learning method tuned for high-throughput sample fabrication

Armi Tiihonen , Chalmers University of Technology

Accelerated materials screening and self-driving laboratories are closely linked to to the development high-throughput (HT) sample fabrication [1]. The umbrella covers a range of techniques from combinatorial chemistry with, e.g., microplates or microfluidic systems, to printers such as inkjet or 3D printers [2], and deposition techniques, e.g. physical vapour deposition. Another take on accelerating materials screening is to guide sampling toward promising compositions. Bayesian optimization (BO) machine learning method, originally designed for sample-efficient optimizations of black-box functions, is frequently used for this purpose [3].

Integrating the two approaches -- HT sample fabrication and BO -- risks, however, losing their mutual benefits. BO samples sequentially one sample at a time, or batches of samples, across the compositional search space. The larger the batch size, the further BO deviates from the optimal information gain achieved via single-sample batches. Similarly, the high throughput in HT fabrication is diminished if BO suggests batches that cannot be fabricated without arduously re-loading the equipment between the requested samples -- e.g., with new stock solutions, ink cartridges, or material targets. We introduce a line-gradient BO method that solves this incompatibility with high-throughput sample fabrication setups and benchmark it in simulated 10-dimensional optimizations, where the line-gradient BO overperforms the traditional BO.

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Keywords

Bayesian optimization, high-throughput fabrication, materials screening

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The nanopowder synthesis and ceramics sintering of Mg1–xAxAl2O4 (A = Zn, Ca, Sr, Ba) spinels and their structure peculiarities study

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Leonid Vasylechko , Lviv Polytechnic National University, Lviv, Ukraine
Vitalii Stadnik , Lviv Polytechnic National University, Lviv, Ukraine
Yulia Rumiantseva , Łukasiewicz Research Network – Krakow Institute of Technology, Krakow, Poland
Yaroslav Zhydachevskyy , Institute of Physics, Polish Academy of Science, Warsaw, Poland

Optical transparency from the UV to IR range of the spectrum, along with other attractive properties of $MgAl_2O_4$ spinel, accounts for its widespread use as an optical material for lasers, optical windows and phosphors. The crystal structure of $MgAl_2O_4$ spinel is formed by densely packed oxygen atoms, which form a rigid structural framework with tetrahedral and octahedral voids, the number of which exceeds the number of cations occupying them. This feature determines the high mobility of cations and, in particular, the high radiation resistance of spinel compounds and their ability to recover from damage after intense irradiation.

This work is devoted to studying the influence of Mg cation substitution for Zn, Ca, Sr, Ba on the features of the spinel-type crystal structure, as well as attempts to produce transparent ceramics by high-pressure high-temperature (HPHT) sintering of nano- and micro-powders synthesized by various methods and annealed in the range from 800 to 1200 °Cin air. We have found that only Zn substitution forms a solid solution $Mg_{1-x}Zn_xAl_2O_4$ across the entire range of x = 0...1. Accurate estimates of the crystal structure parameters showed that $MgAl_2O_4$ initially crystallises with an inverted cation distribution and becomes normal with increasing annealing temperature, unlike $ZnAl_2O_4$, which crystallises immediately with normal ordering. Other substituting cations retain the cubic structure of spinel only at a limited level of substitution.

Keywords

spinel, crystal structure, inversion, solid solution

Acknowledgements

The study has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 EUROfusion). This work was co funded by the Polish Ministry of Science and Higher Education within the project “Development of a technology to produce transparent spinel for optical applications” (No. 602430).

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ALD on supercapacitor electrodes and their electrochemical behavior

Remuel Isaac Vitto , Tampere University Foundation sr

Activated carbon (AC) is the most widely used supercapacitor electrode for its rapid charge transfer kinetics, long cycling lifetime, and low-cost. However, ACs suffer from limited energy density because its electric-double layer capacitance (EDLC) stores energy at only the electrode/electrolyte interface through ion adsorption/desorption. Atomic layer deposition (ALD) technique offers an effective strategy to overcome these limitations by depositing uniform and conformal ultrathin transitional metal oxide (TMO) films that preserves the high-surface area AC porous structure. Unlike traditional high loading TMO deposition methods with non-uniform and unpredictable film thickness that significantly reduces the AC surface area and electrochemical performance, ALD allows atomic-scale precision over the film thickness to minimize the adverse effects. An ALD cycle involves a four-step process of sequential gaseous precursor pulsing each followed by an inert gas purging to get rid of the excess precursors and by-products. Due to the self-limiting nature of each precursor pulses, a one atomic layer-by-layer growth is ensured and the number of ALD cycles controls the film thickness. The TMO film provides a highly pseudocapacitive behavior that combines fast surface-redox and slow ion-intercalation with the EDLC. The ALD-coated TMO boosts the AC electrochemical performance with an efficient energy storage mechanism that delivers up to approximately twice the specific capacitance and energy density of a bare AC. Overall, these improvements highlight ALD as a promising surface engineering strategy to enhance AC-based supercapacitor electrodes and unlock their potential for the next-generation energy storage devices.

Keywords

Activated carbon, atomic layer deposition, transitional metal oxides, supercapacitor

Synthesis of biomass-based activated carbons for electrochemical applications

Aleksandrs Volperts , Latvian State Institute of Wood Chemistry

Aivars Zhurinsh , Latvian State Institute of Wood Chemistry

Cheap and readily available alternative to the expensive platinum cathode materials of fuel cells are required, and wood based chemically doped activated carbons can be a key to rectify not only this problem, but be applied as electrodes in supercapacitors, offering high surface area (up to 2800 m^2 g^{-1}), excellent capacitance (up to 265 F g^{-1}), and cost-effective scalability for rapid energy storage and release. Biomass-based precursors have hierarchical structure, which can contribute into the formation of the porous materials in the course of activation process, and thus tailored for the further application of the synthesized carbons as electrodes in supercapacitors, for oxygen reduction reactions in fuel cells, hydrogen evolution reactions, or as catalysts or catalyst substrates for other processes.

This study is devoted to synthesis of nanoporous activated carbons with high specific surface on the base of wood chars prepared from alder, birch, oak and eucalyptus, as well as pulping residue black liquor. Activation was made by treatment activation with NaOH at various temperatures to optimize the process in terms of specific surface area pore size distribution.

The relationship of various carbons properties and specific capacitance have been established, and columbic efficiency, leakage current and rate capability of supercapacitors with electrodes prepared from various wood species were determined and discussed.

Keywords

activated carbons, biomass, supercapacitors, catalysts, fuel cells

Femtosecond Laser Treatment of Graphene for Gas Sensing Applications

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Martin Vondráček , Institute of Physics of the Czech Academy of Sciences
Valter Kiisk , Institute of Physics, University of Tartu, Tartu, Estonia
Jaroslav Otta , Institute of Physics, University of Tartu, Tartu, Estonia
Artjom Berholts , Institute of Physics, University of Tartu, Tartu, Estonia
Raivo Jaaniso , Institute of Physics, University of Tartu, Tartu, Estonia

The development of chemically active graphene surfaces is essential for enhancing the performance of next-generation chemiresistive gas sensors, particularly in terms of sensitivity and selectivity. Graphene's unique structure provides a versatile platform, but controlled introduction of defects and chemical modification requires the development of specialized methods.

Laser functionalization offers a precise, contactless, and maskless approach for defect engineering, enabling spatially selective surface modification. A femtosecond laser's ultra-short pulses (pulse durations on the order of 10^{-15} s) can induce structural defects and facilitate the formation of functional groups on CVD graphene without excessive thermal damage to surrounding areas.

Graphene was irradiated with a femtosecond laser in different gaseous environments: ambient air, dry nitrogen, and ethanol vapors carried by nitrogen. Raman spectroscopy confirmed that both the nature and density of the induced defects strongly depend on the treatment atmosphere, with the highest degree of functionalization observed in the ethanol-containing environment. XPS analysis of the ethanol-treated samples was done to clarify the origin of the surface modifications. These findings highlight the potential of laser treatment to tailor graphene surfaces, with promising applications in gas sensor technology and related fields.

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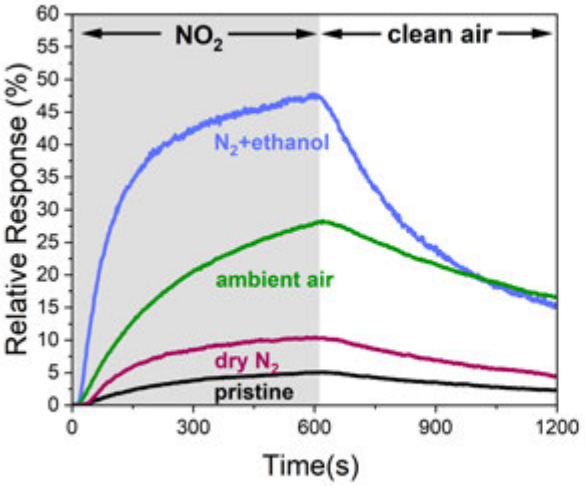
Keywords

Graphene, femtosecond-laser treatment, defects, functionalization, gas sensor

Acknowledgements

This work was supported by the Estonian Research Council grants PRG1580 and TEM-TA 110.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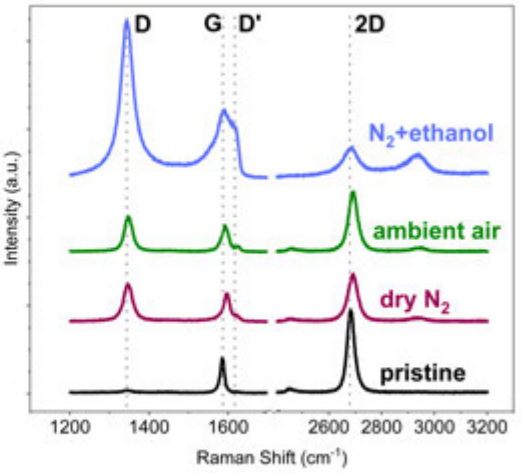
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Liquid Metal Nano-Interface Engineering for Waste-to-Energy Storage Applications

Ali Zavabeti , RMIT University, RTU

Liquid metals and their highly dynamic surface and interface chemistry have recently emerged as powerful platforms for low-dimensional material synthesis and interfacial nanoengineering. The presence of self-limiting oxides, fast atomic diffusion, and reconfigurable liquid surfaces enables unique reaction environments that are difficult to achieve in conventional solid-state systems. As a result, liquid-metal-derived two-dimensional (2D) materials and hybrid nanoarchitectures are gaining strong momentum in sensing, electronics, and energy technologies. Beyond materials harvesting, these adaptive interfaces offer significant opportunities for sustainable chemical transformations and circular-economy strategies.

Here, we report a liquid-metal-enabled nanochemical pathway that converts carbon dioxide (CO_2) and polytetrafluoroethylene (PTFE) waste into functional carbon-based nano-interfaces for energy storage. The approach exploits reaction–diffusion processes at the surface of liquid gallium–lithium (Ga–Li) alloys, where dissolved lithium dynamically migrates to the liquid interface and drives selective reactions under mild, near-ambient conditions.

Within this reactive liquid environment, CO_2 is transformed into interfacial carbonaceous structures, while PTFE undergoes controlled defluorination to yield amorphous carbon and lithium fluoride that self-organise at the liquid metal surface. These coupled processes produce a conformal, electronically coupled nano-interface with high surface area and short ion-transport pathways. The resulting structures can be directly used as binder-free supercapacitor electrodes, highlighting liquid metals as adaptive nano-reactors for sustainable waste-to-energy material platforms.

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Keywords

Liquid Metals, Gallium, Surface Nano-interfaces, Waste to Energy Storage

Acknowledgements

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Collagen–SPION Magnetic Nanocomposites for Small-Scale Oil Spill Remediation in Water Basins

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Gunars Bajars , Institute of Solid State Physics, University of Latvia
Ansis Mezulis , Institute of Solid State Physics, University of Latvia

Latvia has a long coastline and ten seaports. The vessels that work at ports operate on diesel, which occasionally have fuel or motor oil leaks. These oil spills in ports and rivers cause long-term ecological damage despite their limited spatial extent. Latvia also hosts several protected natural water reserves, where maintaining high water quality is crucial important. This project aims to develop an environmentally friendly magnetic adsorbent based on superparamagnetic Fe_3O_4 nanoparticles (SPIONs) stabilized by collagen derived from animal and fish processing waste, following circular economy principles.

SPION–collagen nanocomposites were synthesized starting from dried collagen powder and citric-acid-treated iron oxide nanoparticles. The collagen coating ensured hydrophobic/oleophilic surface properties and improved hydrothermal stability compared to pure collagen. Structural characterization was performed by XRD and Raman spectroscopy [1,2].

Oil adsorption experiments have been performed in controlled laboratory conditions using various oil products (TRL4). The nanocomposite has been dispersed over the oil film and collected by an external magnetic field. Synthesized material demonstrates stable magnetic response and efficient oil capture. Removal of a medium-sized oil spot (1–10 m in diameter) requires, depending on the oil product, 1–2 g/m^2 of adsorbent, and complete collection can be achieved within 10–20 minutes under magnetic guidance.

The material remained magnetically recoverable after repeated cycles, indicating potential reusability. These results confirm successful synthesis and demonstrate enhanced oil removal performance, supporting further validation at TRL5 in a controlled pool environment. The developed approach offers a cost-effective and sustainable solution for rapid remediation of localized oil spills in calm water basins.

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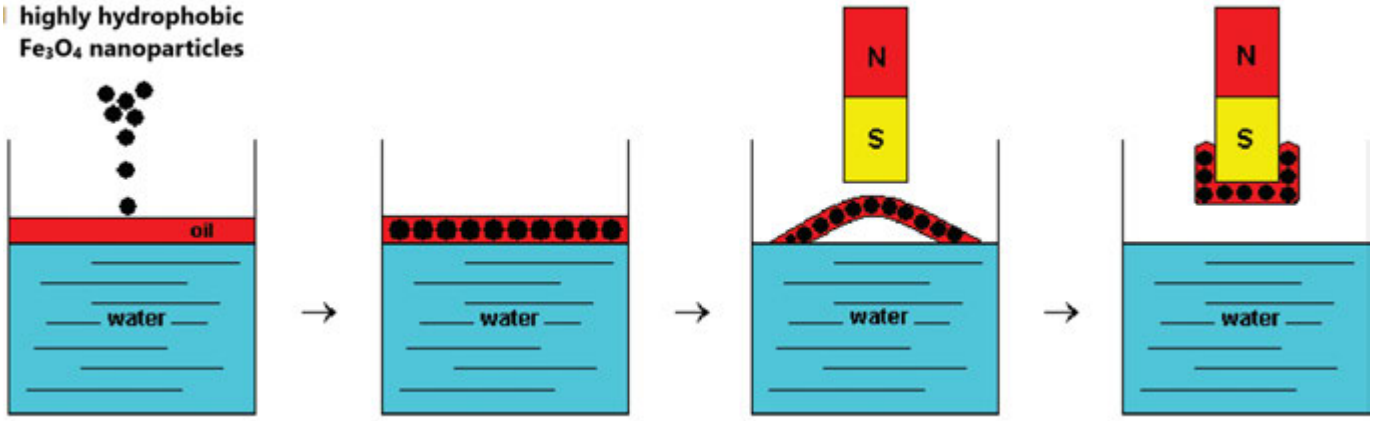
Keywords

oil spill, magnetic adsorbent, hydrophobic and oleophilic nanoparticles, collagen shell, SPIONs

Acknowledgements

This work has been supported by Latvian Council of Science, Fundamental and Applied Research Project: lzp-2025/1-0464



Trap states engineering to improve the persistent luminescence performance of LiGa5O8 spinel-based phosphors

Yaroslav Zhydachevskyy , Institute of Physics, Polish Academy of Sciences

Lithium-gallium spinel ($LiGa_5O_8$) activated with rare-earth (RE) or transition metal (TM) ions is a known crystalline phosphor having long-lasting persistent luminescence (PersL) or mechanoluminescence (ML) properties. In particular, when activated with Cr^{3+}, it exhibits persistent luminescence in the deep red spectral region at about 700 nm. The radiation storage properties allowing the PersL or ML of the material are caused by intrinsic point defects, such as cation antisites, cation and oxygen vacancies that are highly probable in this spinel compound (see e.g. [1]). Recently, we have shown the possibility of tuning the optical band gap, crystal structure and persistent luminescence performance of Cr^{3+}-doped $LiGa_5O_8$ spinel by partially replacing Ga with Al and/or In [2]. The present work aims to go further and to get a better insight into the nature of the intrinsic point defects responsible for the charge trapping and their targeted modification with the purpose of improving the PersL properties of the $LiGa_5O_8$-based phosphors. For this purpose, a few series of $LiGa_5O_8$-based compounds with different Li/Ga ratios, nominally undoped as well as doped with Cr^{3+} or Ce^{3+} ions, have been synthesised by the solid-state reaction method and characterised in detail using powder XRD and luminescence techniques. The obtained results demonstrate that the modification of the $LiGa_5O_8$ host lattice by the Li excess, together with a partial substitution of Ga by Al and In has a high potential for tuning and improving the PersL properties of the material.

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Keywords

Lithium-gallium spinel, persistent luminescence, trap states, crystal structure

Acknowledgements

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Single Photone source and its development in Latvia

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Aivars Vembris , Institute of Solid State Physics, University of Latvia
Arturs Bundulis , Institute of Solid State Physics, University of Latvia
Kaspars Traskovskis , Riga Technical University
Lorenzo Pavesi , University of Trento
Christophe Couteau , University of Technology of Troyes

Single-photon sources are a cornerstone of modern quantum technologies, enabling applications in quantum communication, quantum computing, quantum metrology, and fundamental tests of quantum mechanics. An ideal single-photon source should provide on-demand emission of indistinguishable photons with high purity, brightness, and efficiency, while being compatible with scalable fabrication platforms. In addition, sources capable of generating entangled photon pairs are essential for quantum networking and photonic quantum information processing.

This talk provides an overview of single-photon and entangled-photon sources. More emphasis will be placed on organic emitters, which are attractive due to their narrow optical transitions at cryogenic temperatures, chemical tunability, and compatibility with large-area and low-cost fabrication techniques. The activities of the Institute of Solid State Physics in the field of organic single-photon sources will also be discussed.

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Keywords

Quntum photonics, single photon source, organic molecules

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ABSTRACTS

of the POSTER PRESENTATIONS

Alphabetically by Corresponding Authors

Technologies and Devices

Preperation and Photochromic Properties of Hybrid Co-doped TiO2/amino-PDMS Gels

Loreta Abricka , Riga Technical University

Raivis Eglītis , Institute of Physics and Materials Science, Faculty of Natural Sciences and Technology, Riga Technical University
Andris Šutka , Institute of Physics and Materials Science, Faculty of Natural Sciences and Technology, Riga Technical University

Photochromic materials offer great ways for passive smart window applications. Because of their ability to change their light transmittance in visible and/or infrared light spectra, smart Windows can function as energy or privacy management systems[1].

Titanium dioxide (TiO_2) has proven itself as a viable alternative of inorganic photochromic materials (such as WO_3, V_2O_5 and NiO), due to its strong photochromic response, stability and, importantly, low cost and non-toxicity[2]. However, the photochromic effect of TiO_2 is achieved only in the presence of a hole scavenger. This limits its practical use, as it complicates the system design and prevents sufficient long-term effect due to the eventual hole scavenger exhaustion. Recently, it has been reported that this problem can be overcome through co-doping TiO_2 with Nb^{5+} and Hf^{4+} ions. Results show photodarkening of the modified nanoparticles without any additional hole scavengers present, thus making these nanoparticles more suitable for use in smart window technologies[3].

The next step towards smart window applications is the integration of the co-doped TiO_2 nanoparticles into a gel matrix. This can be achieved by incorporating the nanoparticles inside an amino-functional PDMS, obtaining a gel-like organic/inorganic structure. These structures have successfully exhibited reversible photochromism in ambient conditions.

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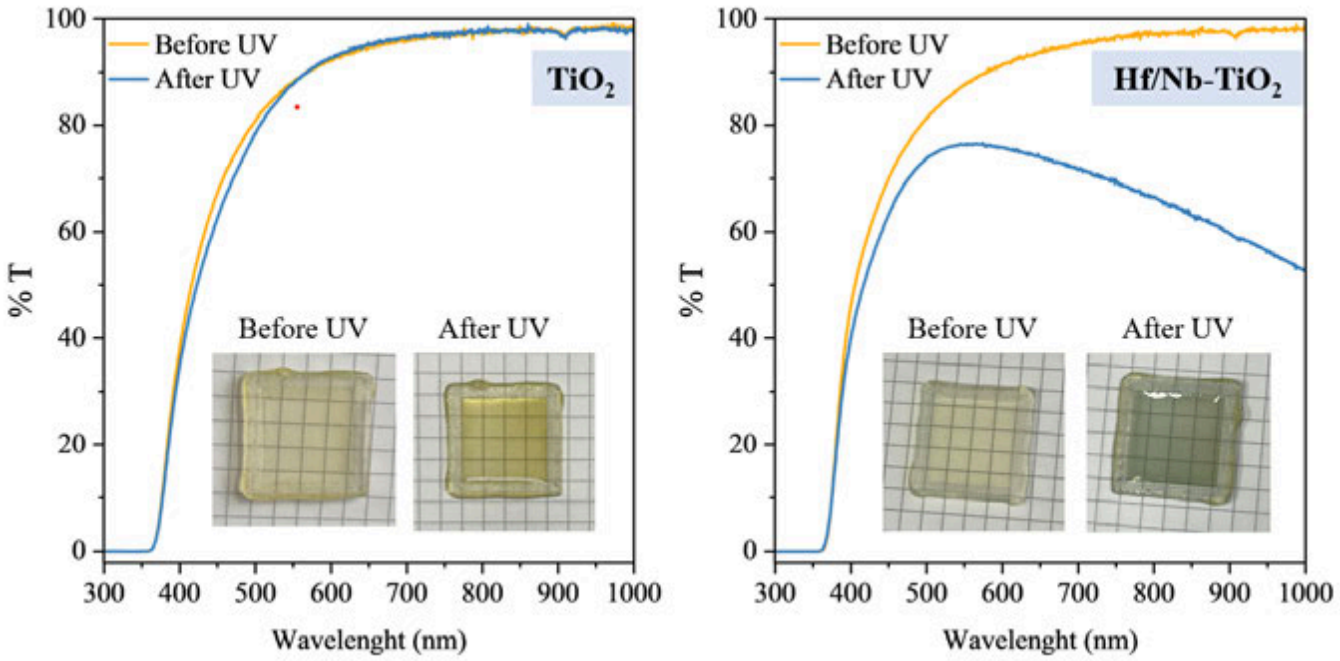
Keywords

Titanium dioxide, Photochromism, Organic-inorganic gel

Acknowledgements

This research was supported by the M-ERA.Net funding mechanism (Project “Smart window based on surface-active thermally responsive hydrogel” (GELWIN)).



Materials for Energy, Theoretical Modeling of Functional Materials and Devices, Technologies and Devices

Comprehensive analysis regarding the development of flexible and ultra-light PEM fuel cells through the integration of advanced nanomaterials for wearable electronics

Marinoiu Adriana , National R&D Institute for Cryogenic and Isotopic Technologies, 240050 Ramnicu Valcea

This study presents the development and performance evaluation of an **improved Membrane Electrode Assembly (MEA)** utilizing **Nitrogen-doped Reduced Graphene Oxide (N-rGO)** as a high-performance catalyst support for Proton Exchange Membrane Fuel Cells (PEMFCs). Traditional MEAs often face limitations due to the high cost of platinum and the electrochemical instability of conventional carbon supports, which are prone to corrosion and catalyst agglomeration.

By introducing N-rGO into the catalyst layer, the nitrogen atoms introduces localized defects and modifies the electronic structure to the carbon framework of the graphene lattice, creating high density active sites that facilitate the Oxygen Reduction Reaction (ORR). Experimental results indicate that the N-rGO architecture significantly enhances the **electrochemical surface area (ECSA)** and promotes a more uniform distribution of Pt nanoparticles, allowing for a substantial reduction in total noble metal loading without sacrificing power output.

Furthermore, the structural integrity of the N-rGO framework provides superior **corrosion resistance** under high-potential operating conditions. The results demonstrate that N-rGO is a promising catalyst support for next-generation PEMFC systems, offering a viable pathway toward high-performance, cost-effective, and sustainable fuel cell technologies.

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Keywords

electrocatalyst; nitrogen-doped graphene oxide; metal-free; long-term operation stability

Acknowledgements

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Materials for Energy, Technologies and Devices

Integrated micro-hydrolysis system of sodium borohydride for powering flexible electronic devices

Marinoiu Adriana , National R&D Institute for Cryogenic and Isotopic Technologies, 240050 Ramnicu Valcea

The paper studies the development of a cartridge-type system containing a $NaBH_4$ solution and a catalytic microreactor capable of releasing high-purity hydrogen. Unlike methanol reforming, $NaBH_4$ hydrolysis does not require high temperatures (it operates efficiently at 27–80°C), making it ideal for devices worn directly by the user (wearables).

This paper addresses two important aspects for providing design data: (i) **Smart micro-dosing** – in this regard, the introduction of a piezoelectric element or a peristaltic pump is proposed to precisely control the flow of solution to the catalyst, allowing hydrogen to be generated only on demand; (ii) **Evaluation of non-precious catalysts** – particularly catalytic systems based on alloys of cobalt, nickel, or boron, optimized to prevent clogging with sodium metaborate.

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Keywords

flexible PEM fuel cells; catalytic microreactor; smart micro-dosing

Acknowledgements

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Materials for Energy, Technologies and Devices

Micro-Reactor Architecture with Capillary Separation and Multidirectional Phase Management

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For a portable device, the orientation of the reactor changes constantly (in a pocket, backpack, or hand). The main challenge in using $NaBH_4$ hydrolysis is that the byproduct, sodium metaborate ($NaBO_2$), is a viscous aqueous solution that can “flood” the outlet port or connection, or block hydrogen flow.

This study focuses on the development of an innovative design based on selective capillarity and hydrophobic membrane-based phase separation. Two gravity-independent separation mechanisms are investigated.

Case 1: The system uses surface tension forces instead of gravity to manage the phases (liquid vs. gas). At the center of the reactor is a 3D porous structure (e.g., nickel foam or 3D-printed polymer) coated with catalyst. This structure “draws in” the $NaBH_4$ solution via capillary action, ensuring proper contact regardless of tilt angle.

Case 2: Another proposed approach involves the use of specific membranes. The outer walls of the reaction chamber are lined with a highly hydrophobic expanded PTFE (Teflon) membrane. The membrane pores allow hydrogen molecules to pass through while completely blocking the aqueous solution and liquid byproducts, even under moderate pressure.

To prevent the accumulation of $NaBO_2$ (which can crystallize and clog the reactor), the design includes conical evacuation channels. The micro-outlet channels have a divergent geometry. The Laplace pressure difference naturally drives the spent liquid toward a peripheral collection reservoir, effectively “cleaning” the active catalytic zone.

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Keywords

H2 catalytic microreactor; selective capillarity; hydrophobic membrane-based phase separation

Acknowledgements

This work was supported by the project PN 23 15 01 03, Contract No. 20N/2023, Core Program within the National Research Development and Innovation Plan 2022-2027, financed by Ministry of Research, Innovation, Digitization of Romania and by the project RO-HydroHub “Romanian Hydrogen and New Energy Technologies Hub”, contract nr. G2025-113330/ 2025, SMIS code: 351358, finaced from European funds via the POCIDIF 2021-2027 Program, activity “A4.4 Industrial – level research for flexible fuel cells development”.

Ferroelectrics and Functional Materials

Formation mechanism of core–shell structures in lead-free ferroelectric ceramics via the diffusion method.

Gusts Agafonovs , Institute of Solid State Physics, University of Latvia

The development of high-performance lead-free ferroelectrics remains a key challenge as the field continues to seek alternatives to Pb-based materials. One promising approach to improving their functional properties is the formation of core–shell type microstructures, however, the ability to controllably create such structures in bulk ceramics is still limited. In this study, a method is introduced that enables the formation of core–shell structures in fully sintered lead-free ceramics, including $BaTiO_3$ (BT), $SrTiO_3$ (ST), $Na_{0.5}Bi_{0.5}TiO_3$ (NBT), and ZnO. The method is based on thermally treating two polished ceramic plates placed in direct contact, which promotes elemental diffusion along grain boundaries. In all investigated combinations, NBT acts as the primary diffusion source, while Bi overstoichiometry in its composition further enhances both the diffusion intensity and the penetration depth. The fact that the ceramic plates remained detachable after thermal treatment indicates that elemental transfer between them occurs through the vapor phase. Independent studies on the thermal treatment of NBT ceramics show that volatilization takes place predominantly within a thin surface layer. Thermogravimetric data further confirm that NBT with excess Bi exhibits a substantially higher vapor pressure than stoichiometric NBT, which explains the more pronounced formation of core–shell structures in the presence of Bi overstoichiometry.

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Keywords

lead free ferroelectric ceramics, core–shell, diffusion

Acknowledgements

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Materials for Photonics

Charge trapping and persistent luminescence in alkaline earth metal pyrophosphates

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Alkaline earth phosphates readily accommodate a large variety of intrinsic and dopant-induced point defects, which play a central role in many optical properties. Motivated by recent reports of highly efficient persistent luminescence in selected rare-earth ion-doped phosphates [1-3], we systematically investigate radical formation, charge trapping, and persistent luminescence in Pr-doped alkaline earth pyrophosphates, $X_2P_2O_7$ (X = Ca, Sr, Ba). Electron paramagnetic resonance (EPR) spectroscopy is applied to characterise radicals that form during X-ray irradiation. The origin of several phosphorus-related radicals is proposed based on ^{31}P hyperfine couplings determined from multifrequency spectra simulations. Stepwise annealing experiments are correlated with thermally stimulated luminescence (TSL) measurements to identify the dominant defects contributing to radiative recombination processes. The best-performing pyrophosphate persistent phosphor is identified based on luminescence radiance measurements.

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Keywords

Phosphate, electron paramagnetic resonance (EPR), persistent luminescence

Acknowledgements

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Technologies and Devices

Carrier transport in CVD graphene field-effect transistors

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Since the discovery of graphene, there have been extensive studies in two-dimensional materials research [1,2]. Electrical properties of graphene such as noise and current-voltage characteristics were explored [3]. The goal of this work is to investigate carrier transport in back-gated graphene field-effect transistor structures. The samples were prepared using CVD monolayer graphene on Cu. Then the graphene film was transferred to 100 nm SiO_2/p-Si wafers [4]. To define the active channel, the graphene was patterned using photolithography to form TLM patterns with lengths L = 5-20 μm and widths w = 5-40 μm. Lastly, Ti/Au contact metals were deposited. Current-voltage characteristics were measured both in DC and pulsed (from 5 ns to 1.1 μs) regimes at room temperature. The carrier drift velocity was estimated from the data on pulsed current density and the constant carrier density. The graphene current transfer and output characteristics showed the presence of p-type type graphene channel. From the transfer characteristics the estimated graphene channel field-effect mobility was ~700 cm^2/Vs. The graphene mobility and channel resistance values gave hole density of $9.1x10^{12}$ cm^{-2}. The room temperature t = 5 ns duration pulsed current density-electric field and velocity-electric field characteristics are illustrated in Figure 1. The resultant highest hole drift velocity of $6.5x10^6$ cm/s is estimated at ~12 kV/cm and can be associated with the influence of non-equilibrium optical phonons [5].

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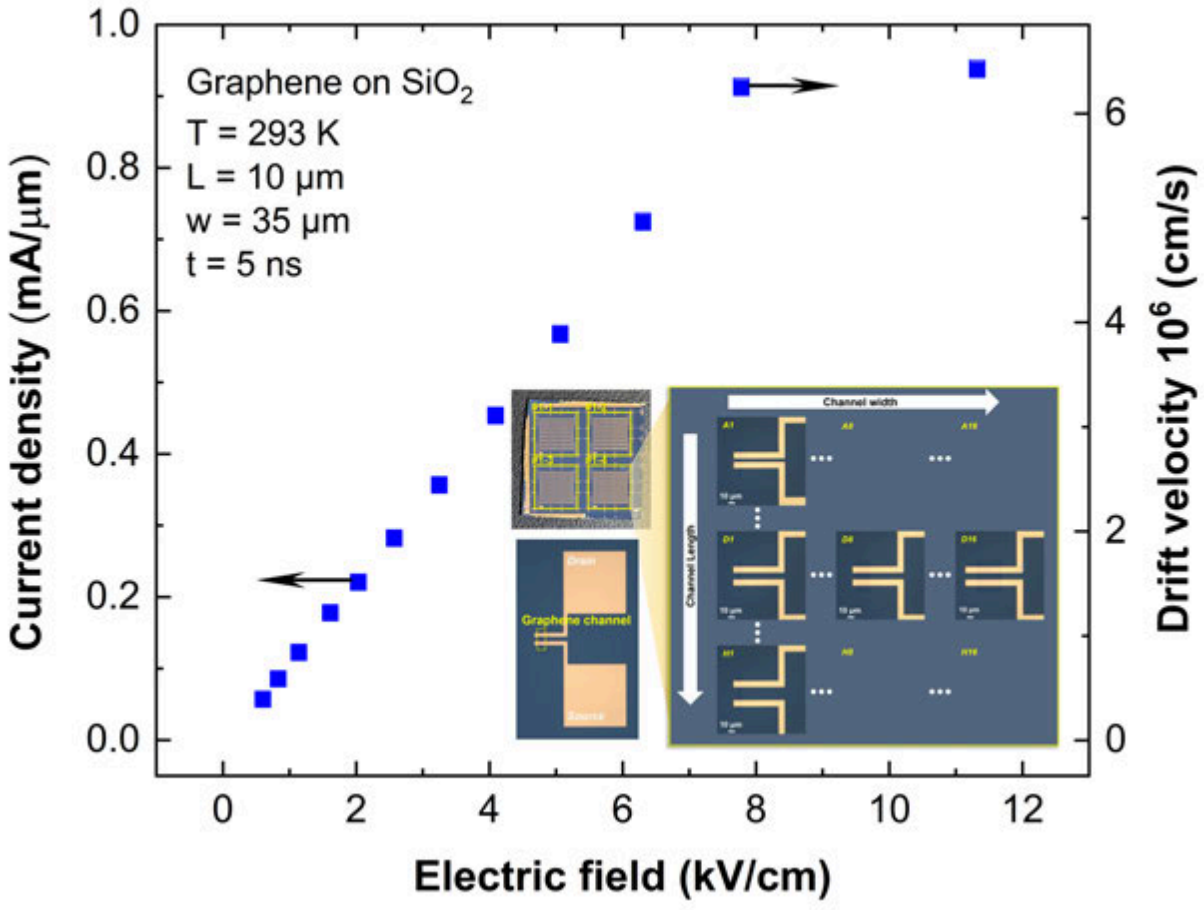
Keywords

graphene FET; electric field; ns-pulsed current-voltage characteristics; carrier drift velocity



Materials for Energy

Thermal properties for radiation-modified sheep wool fibers

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In the recent years changes in agricultural and farming habits, including the trends of cultivation of lands in uneven terrains is taking place. Sheep farming has strategic importance in achieving long-term agricultural resilience [1]. However, in the recent years the sheep wool becomes a challenging aspect due to the complex disposal management [2]. Therefore, implementation of the sheep wool fibers into various composite materials, pretreatment for improvement of properties, and finding novel approaches for using waste sheep wool is crucial for the creation of environmentally friendly materials and sustainable development [3].

In the present research, sheep wool fibers from local, Latvian Blackhead sheep breed were characterized using Fourier transform infrared and electron paramagnetic resonance (EPR) spectroscopy before and after irradiation with accelerated electrons. Thermal properties were analysed by thermogravimetry/differential scanning calorimetry.

Thermally induced decomposition of sheep wool takes place in three main steps, where the first, up to 100 °C is related with water desorption, in the range of 200-400 °C degradation of -NH bonds takes place, while starting from 400 °C intense oxidation together with release of CO_2 occurs. Several effects, such and dependency on irradiation dose and irradiation atmosphere were observed. EPR spectra indicate to the radiation induced formation of paramagnetic centres on sulphur and carbon atoms takes place.

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Keywords

Sheep wool, irradiation, thermal properties

Acknowledgements

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Materials for Photonics

Atypical Near-Infrared Photochromism in Samarium-Doped Hackmanite

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Hackmanites are materials known for their diverse optical properties, including tenebrescence – colour change under ultraviolet radiation. Their composition can be fine-tuned with minimal synthesis adjustments to modify their optical properties.

It is well documented that these materials can be doped with lanthanides for traditional luminescence applications, such as LEDs. However, in this study, we investigated the influence of lanthanides, specifically samarium, on the photochromic properties of the material. In this research, lanthanide-doped hackmanites were synthesised via a solid-state route using Ln^{3+}-doped lithium aluminosilicates ($LiAlSiO_4$) as the starting material, rather than the commonly employed zeolite A. The samples were characterised by X-ray diffraction (XRD) and confirmed to be pure.

Utilising Sm^{3+} as the lanthanide dopant resulted in a hackmanite exhibiting an unconventional photochromic response, characterised by absorption extending into the near-infrared region and a predominance of thermal bleaching. Although the precise details of the tenebrescence mechanism remain not fully understood, spectroscopic evidence indicates the involvement of Sm^{2+}/Sm^{3+} redox processes in conjunction with disulphide photochromic centres within the tenebrescence mechanism. The findings demonstrate that lanthanide doping can significantly alter the photochromic behaviour of hackmanites, thereby enabling additional functionalities and potential applications.

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Keywords

hackmanite, lanthanide, samarium, photochromism

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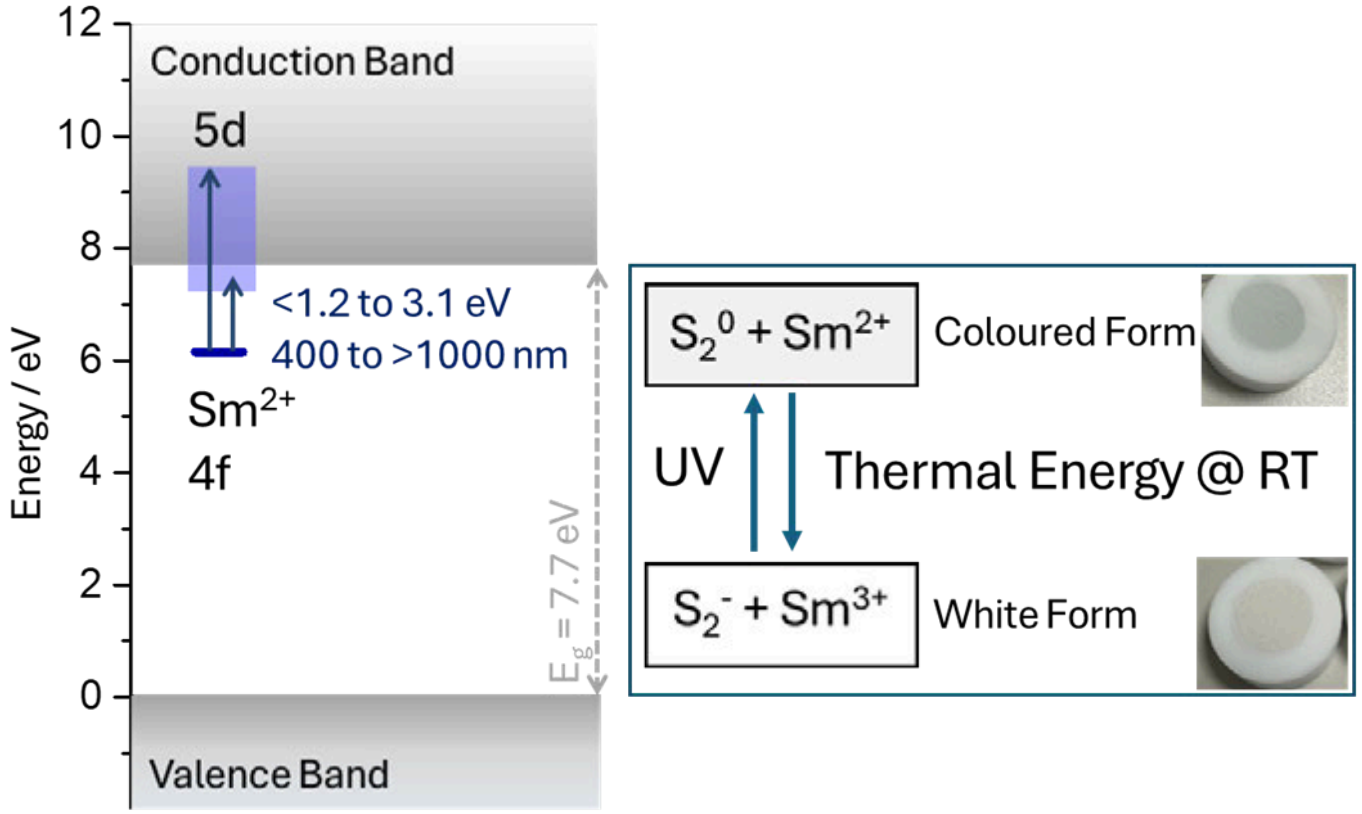

Ferroelectrics and Functional Materials

High-Frequency Magnetic Characterization of CERN Fast Kicker Magnet Materials

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A wide range of magnetic materials, including ferrites, magneto-dielectrics, and multiferroics, are used in accelerator technology. Among these, ferrites are most widely employed due to their high magnetic permeability, particularly in fast kicker magnets for beam injection and extraction in CERN circular accelerators. However, manufacturer data are often insufficient to accurately describe the frequency-, temperature-, and field-dependent properties required for reliable magnet design.

This work presents a high-frequency characterization of magnetic permeability of materials used in CERN fast kicker magnet systems. Measurements were performed using an extended single-turn inductor setup, selected for its simple modeling and reliable calibration. The method captures frequency-dependent behavior associated with spin rotation and domain wall motion, including additional loss mechanisms in the GHz range.

Magnetic permeability was measured for baked and unbaked ferrites over a wide temperature range. Complementary studies were conducted on alumina and laminated steel components. Electromagnetic simulation tools were used to extend the frequency range and improve material parameter extraction. The results provide essential data for the optimization and reliable operation of fast kicker magnets in accelerator environments.

Keywords

magnetic permeability, ferrite, single-turn inductor

Acknowledgements

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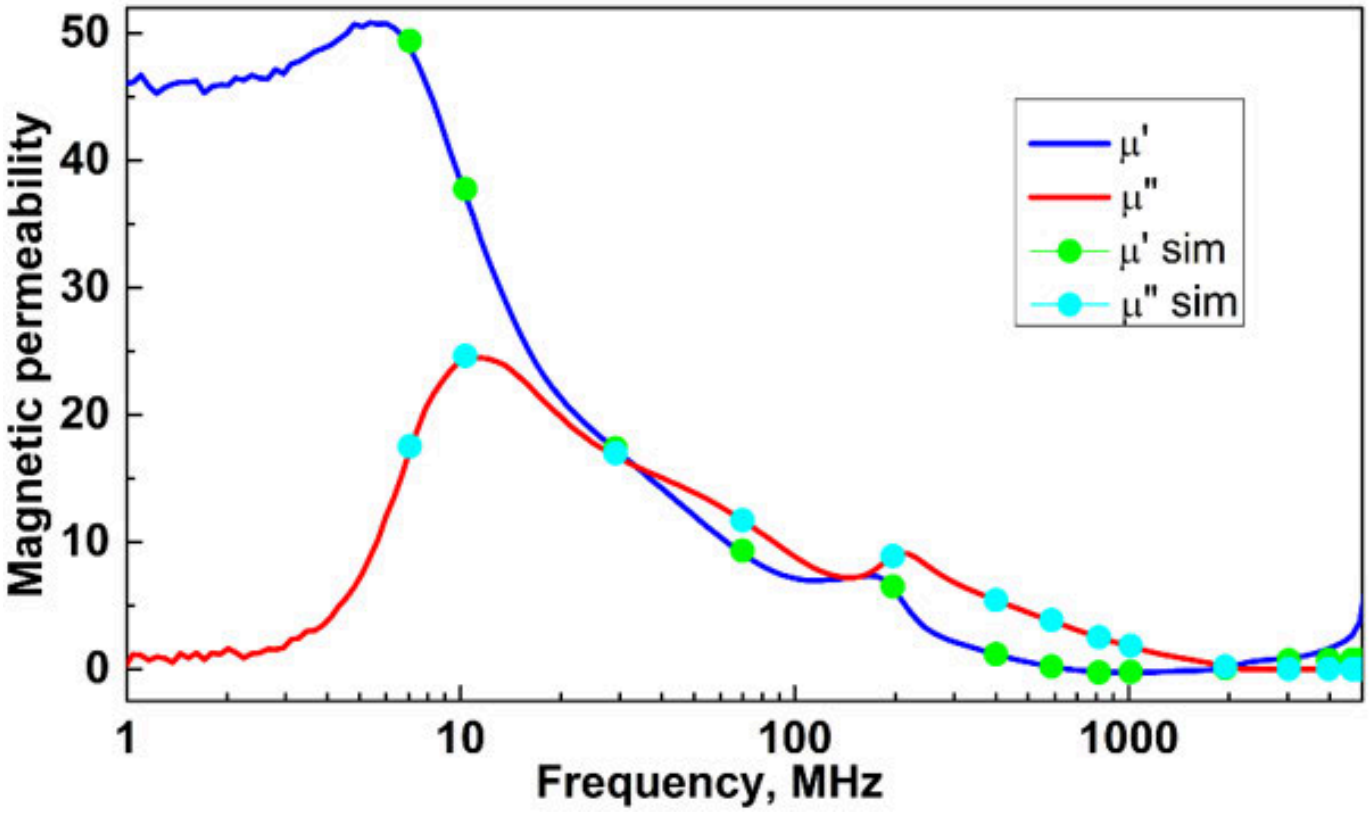
Magnetic permeability
50
40
30
20
10
0
1
10
100
1000
Frequency, MHz
μ'
μ"
μ' sim
μ" sim

Materials for Photonics

Novel Designs of Transparent Microscale Copper Electrodes and Their Impact on Electrochromic Device Performance

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Electrochromic devices (ECDs) are promising for applications requiring dynamic control of optical properties, such as smart windows and displays. In this study, we investigate the performance of ECDs employing copper line electrodes with varying geometries, using PEDOT:PSS and WO_3 as electrochromic materials, and $LiClO_4$ or H_2SO_4 as electrolytes. Copper is evaluated as a cost-effective alternative to conventional transparent conductors, but its stability in different electrochemical environments is a key concern. Devices are systematically characterized in terms of optical modulation, switching speed, and cycling stability. Our results show that electrode geometry significantly influences transmittance and switching kinetics, while the choice of electrolyte critically affects copper stability and overall device longevity. Notably, PEDOT:PSS devices with $LiClO_4$ electrolyte exhibit stable operation with pure copper electrodes, whereas devices using H_2SO_4 show rapid degradation. These findings provide valuable guidelines for the design of high-performance, durable electrochromic devices using copper-based transparent electrodes.

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Transparent microscale electrodes formed by laser-induced metal deposition on glass for smart windows application, Optics & Laser Technology, 2025, 113669. https://doi.org/10.1016/j.optlastec.2025.113669. Laser-induced microscale copper trace deposition on glass and PET substrates, https://doi.org/10.1016/j.optlastec.2024.112355

Keywords

Electrochromic device; copper electrode; PEDOT:PSS; tungsten trioxide; $LiClO_4$; H_2SO_4; electrode geometry; electrolyte compatibility; optical modulation; device stability

Ferroelectrics and Functional Materials

Broad-band dielectric and Raman study of structural transformations in van der Waals ferrielectric CuInP2S6

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Chalcogenide hypothiodiphosphates of $CuInP_2S_6$ family exhibit a combination of ferroelectric, semiconducting and optical properties [1]. The appearance of spontaneous polarization of these ferrielectrics is related to the second order Jahn-Teller effect for copper cations located in a double-well local potential, and to the stereoactivity of indium cations. The indium sublattice anharmonicity dominates below 200 K, which induces the coexistence of the dipole glass and ferrielectric states. Thermal activation of the copper relaxation dynamics results in the formation of a long-range fluctuating clusters of spontaneous polarization above the first order transition temperature $T_c \approx 312$ K into the paraelectric phase. The relaxation dynamics of Cu^+ cations is associated with significant deformations of the $(P_2S_6)^{4-}$ anions, causing buckling of the sulfur sheets at the border with van der Waals gap. The resulting rise of such structural disorder promotes the Cu^+ cations localization inside of this gap, where they bond with sulfur atoms from the neighboring structural layer. Formation of unfilled sulfide octahedra can also lead to the collinear orientation of the electric dipoles of In^{3+} and Cu^+ cations, inducing ferroelectric character of ordering inside of polar clusters state above T_c. By THz time-domain spectroscopy, in comparison to the coaxial dielectric spectroscopy data [2], and together with Raman scattering study, the phonon spectra and relaxation dynamics of $CuInP_2S_6$ across the ferrielectric to paraelectric phase transition are traced. With analysis of the low frequency (20 -70cm^{-1}) and middle frequency (290 - 330 cm^{-1}) spectral bands, the displacements of Cu^+ ions between inside of structural layer and in-gap positions and their coupling with interlayer sliding are characterized.

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Keywords

2D ferroelectrics, Chalcogenide single crystals, Dielectric spectra, Terahertz spectroscopy, Raman scattering

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Materials for Energy

Functional carbon aerogels as electrode materials for sodium-Ion energy harvesting and storage devices

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Development of light-weight, cost-effective, and environmentally-friendly, and safe electrochemical energy storage devices can open a new path to a variety of applications leading to the increase of energy-efficiency of society. From this perspective, Na-ion batteries employing having ultralow density, large surface area, high electrical conductivity and chemical robustness [1] carbon aerogels, are one of the most attractive solutions.

In this work, bare, Na-doped, and P-doped carbon aerogels were investigated as potential electrode materials for aqueous Na-ion batteries. The carbon aerogel electrodes were synthesized via sol–gel polycondensation of resorcinol with formaldehyde, followed by ambient pressure drying and subsequent carbonization. Sodium and phosphorus doping was introduced during the synthesis process to enhance the electrochemical activity and sodium-ion storage capability of the material.

The surface morphology and porous structure of the obtained carbon aerogels were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray diffraction (EDX) spectroscopy. Electrochemical performance was evaluated using electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic charge/discharge (GCD) measurements in a conventional three-electrode cell using a PalmSens4 potentiostat.

The synthesized carbon aerogels exhibited a highly porous interconnected structure with uniform dopant sodium and phosphorus distribution throughout the carbon matrix. Electrochemical measurements demonstrated improved sodium-ion storage performance including enhanced reversible capacity, lower charge-transfer resistance, and stable cycling behaviour. These results suggest that Na-doped and P-doped carbon aerogels are promising candidates for electrode materials in next-generation sodium-ion batteries.

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Keywords

Sodium-ion battery; carbon aerogel; electrode material; aerogel doping; electrochemical characterization

Acknowledgements

The work was performed within the ERDF project No 1.1.1.3./1./24/A/113 “Innovative multifunctional nanomaterials systems for enhancing energy efficiency of building envelope”.

Ferroelectrics and Functional Materials

One-pot intrapore encapsulation of copper species in mesoporous SiO2 nanocomposites for durable antimicrobial surface coatings

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Antimicrobial surfaces are increasingly needed to limit pathogen transmission on high-touch surfaces, which contribute to up to 40% of hospital-acquired infections. Many antimicrobial coatings loose activity under practical conditions. Mesoporous nanocomposite based coatings provide a strategy to address this limitation by confining antimicrobial agents within mesoporous SiO_2 pores, enabling controlled and sustained release. In this work, mesoporous silica nanocomposites were synthesized using a one-pot micelle-templated sol-gel approach that enables direct incorporation of $[Cu(NH_3)_4]^{2+}$ during particle formation, yielding $[Cu(NH_3)_4]^{2+}@SiO_2$ nanocomposites. Subsequent calcination converted the $[Cu(NH_3)_4]^{2+}$ into CuO_x domains, forming $CuO_x@SiO_2$ nanocomposites. Characterization confirmed preserved morphology and no extrapore copper (Figure 1&2).

The $CuO_x@SiO_2$ nanocomposites exhibited diffusion-controlled copper release, and calcination reduced cumulative 24 h leaching of copper, consistent with transformation of $[Cu(NH_3)_4]^{2+}$ complex into confined CuO_x domains within the mesoporous silica. In antibacterial assays against *E. coli*, *P. aeruginosa* and *S. aureus*, both nanocomposites exhibited bactericidal activity and maintained it after 24 h of exposure in deionized water, confirming that sufficient copper species remained confined within the mesoporous framework to support durable antimicrobial activity. Notably, $CuO_x@SiO_2$ was non-cytotoxic to human keratinocyte (HaCaT) cells while maintaining antibacterial performance, demonstrating that intrapore CuO_x confinement enhances stability and biological compatibility for durable antimicrobial surfaces.

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Keywords

Mesoporous silica, nanocomposites, copper leaching, antimicrobial activity

Acknowledgements

Financial support from the Estonian Research Council (PRG1496 and TK210 “Center of Excellence in Sustainable Green Hydrogen and Energy Technologies”), the European Commission project FAST-Real (Grant Agreement ID: 101159721), and the European Union and Ministry of Education and Research via project TEM-TA55 is gratefully acknowledged. The research was partly conducted using the NAMUR+ core facility funded by project TARISTU24-TK26 “Center of nanomaterials technologies and research (NAMUR+).

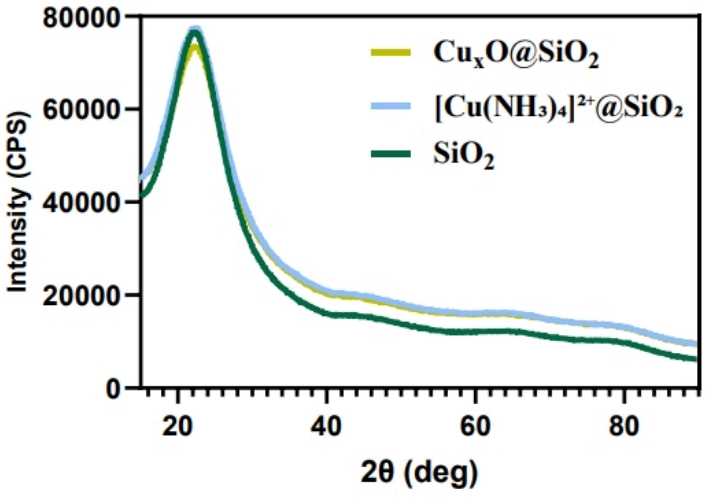

Figure 1. XRD patterns of SiO_2, $[Cu(NH_3)_4]^{2+}$@SiO_2 (1.5%), and Cu_xO@SiO_2 (1.5%).

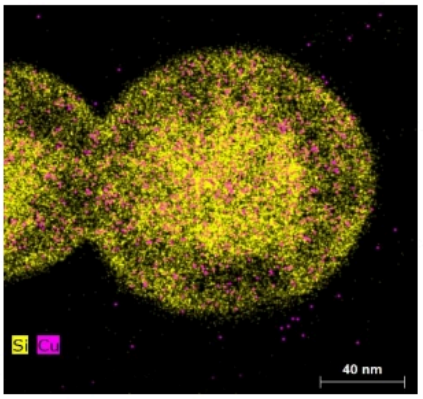

Figure 2. Elemental mapping (40 nm scale) showing uniform distribution of Si (yellow) and Cu (magenta) within spherical nanocontainer.

Technologies and Devices

AFM-Based Electrical Characterization of Doped Indium Oxide Thin Films for Accelerated Material Screening

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This study reviews and compares indium oxide thin films using AFM-based electrical characterization techniques. Amorphous and polycrystalline samples doped with tantalum and germanium were investigated. The motivation behind this work lies in the promising applications of these materials within monolithic 3D integrated devices. However, a trade-off exists between electron mobility and electrical stability when doping the material, as conduction is facilitated by oxygen vacancies. Material development in this direction typically requires device fabrication to measure the impact of the dopants, which is a costly endeavour. In an effort to circumvent this bottleneck, this study directly measures local conductivity using conductive AFM. Although AFM is not a high-throughput method, several properties can be measured simultaneously, such as the dielectric constant, surface charge , surface morphology and conductivity . This provides a framework for an improved material development pipeline that can guide device fabrication towards the most promising material stoichiometries. This proof of principle study focuses on nanoscale impurities and defects within otherwise homogenous samples.

Technologies and Devices

Heteroepitaxial stabilization of α-phase Ga2O3 thin films with superior thermal conductivity compared to β-phase

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Gallium oxide (Ga_2O_3) is an emerging ultrawide-bandgap semiconductor for next-generation power electronics. However, the relatively low thermal conductivity of the technologically most promising β-Ga_2O_3 phase poses a major challenge for thermal management in high-power devices. The metastable corundum α-Ga_2O_3 phase is predicted to exhibit higher thermal conductivity and offers good lattice compatibility with sapphire substrates, making it a promising alternative for improved heat dissipation. In this work, α-Ga_2O_3 thin films were heteroepitaxially grown on m-plane sapphire substrates by reactive pulsed-DC magnetron sputtering from a liquid gallium target [1-2]. A 207 nm thick α-Ga_2O_3 film was investigated and compared with two β-Ga_2O_3 samples: a 500 nm heteroepitaxial film on sapphire grown by metalorganic chemical vapour deposition [3] and a commercial β-Ga_2O_3 epilayer. Structural properties were examined by X-ray diffraction and Raman spectroscopy, while thermal conductivity was measured using time-domain thermoreflectance (TDTR). The α-Ga_2O_3/sapphire heterostructure exhibited the highest thermal conductivity of 22 ± 2 $W{\cdot}m^{-1}{\cdot}K^{-1}$ at room temperature, significantly exceeding the value obtained for the 500 nm β-Ga_2O_3 film on sapphire (3.7 ± 0.2 $W{\cdot}m^{-1}{\cdot}K^{-1}$) and also surpassing the β-Ga_2O_3 epilayer (9.3 ± 0.3 $W{\cdot}m^{-1}{\cdot}K^{-1}$). These results demonstrate the potential of heteroepitaxially

stabilized α-Ga_2O_3 thin films on sapphire as a promising platform for improved thermal management in Ga_2O_3-based power devices.

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Keywords

thin film, gallium oxide, epitaxy, thermal conductivity, metastable phase

Acknowledgements

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Technologies and Devices

Evaluation of Pseudomonas aeruginosa–induced corrosion on antimicrobial high-entropy alloys coatings

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Microbiologically induced corrosion (MIC) represents a critical degradation mechanism for metallic materials exposed to aggressive biological environments. In this study, the corrosion behavior of antimicrobial high-entropy alloy (HEA) coatings was investigated under biotic conditions induced by *Pseudomonas aeruginosa*. Several HEA coatings with different copper contents were evaluated and compared with uncoated 304L stainless steel.

The results revealed that the number of viable bacteria (MPN) ranged between 10^8 and 10^{12} cells/mL, with maximum values recorded for uncoated 304L stainless steel and minimum values for the AlFeCrNiCu coating with high Cu content (16% Cu), confirming the antibacterial effect of copper-rich HEA coatings. After 60 days of exposure, both macroscopic and microscopic surface modifications were observed, with their severity depending on the coating composition and test conditions (biotic versus abiotic). The most significant surface modifications were observed on CuCrFeMnNi (5% Cu) and AlFeCrNiCu (16% Cu, 2.5% Al) coated samples. CuCrFeMnNi (5% Cu) coatings exhibited higher sensitivity, showing degradation under both biotic and abiotic conditions. In contrast, AlFeCrNiCu (16% Cu, 2.5% Al) coatings displayed surface changes only under biotic conditions, indicating superior resistance to abiotic corrosion. These differences are attributed to the chemical composition of the coatings, which influences biofilm formation and interactions with the *Pseudomonas aeruginosa* consortium.

These findings demonstrate that the chemical composition of HEA coatings plays a crucial role in controlling biofilm development and microbiologically induced corrosion mechanisms.

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Keywords

Microbiologically induced corrosion (MIC), High-Entropy Alloy, coatings, Pseudomonas aeruginosa

Acknowledgements

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Materials for Energy

Thermoelectric Properties of Silver-Doped Copper Iodide / PEDOT:PSS Composites

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Hybrid organic-inorganic composites based on conducting polymers are considered promising materials for thermoelectric energy conversion near room temperature due to their intrinsically low thermal conductivity and tunable electrical transport properties. In this work, composite materials based on silver-doped copper iodide (CuI:Ag) and the conductive polymer PEDOT:PSS (Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate) were investigated in the form of both pellets and thin films.

The composites were prepared by incorporating copper iodide particles doped with 15% silver into PEDOT:PSS matrices of different types, including water-based and anisole-based systems, at varying polymer concentrations. The influence of composite composition, polymer matrix type, and sample morphology on thermoelectric performance was analyzed. Electrical conductivity and the Seebeck coefficient dependence on the temperature were measured, and thermoelectric efficiency was evaluated through the power factor.

The obtained results demonstrate that the thermoelectric properties of the composites strongly depend on the polymer content and morphology of the samples. These findings indicate the potential of CuI-based polymer composites as promising materials for thermoelectric applications near room temperature.

Keywords

thermoelectric properties, PEDOT:PSS, Seebeck coefficient, electrical properties

Acknowledgements

This research was funded by the Latvian Council of Science, grant number LZP-2023/1-0456 “Advancing Sustainable Thermoelectric Hybrid Systems Utilizing Glass-Forming Low Molecular Weight Compounds”.

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Real-time Automated Identification and Quality Assessment of 2D Materials using Referring Expression Segmentation

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The fabrication of high-quality two-dimensional (2D) materials is critical for advanced applications in nanophotonics and integrated circuits. However, existing production methods—such as Chemical Vapor Deposition (CVD) and mechanical exfoliation—suffer from contamination risks and inconsistent quality. Current post-fabrication assessment relies heavily on subjective manual inspection, which acts as a bottleneck for efficient manufacturing.

In this work, we present an automated deep learning framework designed to streamline the evaluation of 2D material monolayers. By leveraging Referring Expression Segmentation (RES) combined with a bidirectional cross-modal fusion module, our model effectively integrates visual and semantic cues to achieve high-precision boundary detection. Beyond segmentation, we introduce a "Successful Label" classification mechanism to automate the assessment of material usability, significantly reducing dependency on expert judgment.

Our system has been successfully integrated to real-time recognition via optical microscopy. This end-to-end solution provides a standardized, efficient workflow for 2D material processing, demonstrating its potential for real-world manufacturing and experimental research.

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Keywords

Two-dimensional Materials, Referring Expression Segmentation, Binary Classification

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Theoretical Modeling of Functional Materials and Devices

Computational study of the structural, electronic, vibrational and elastic properties of Na_2SiF_6 and Na_2SiF_6:Mn4+ phosphors

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Red-emitting crystalline phosphors are materials that emit intense red light when excited by an external energy source, such as ultraviolet or blue radiation. Alkali hexafluorosilicates with the general formula A_2SiF_6 are considered promising phosphor materials, since their structures contain $[SiF_6]^{2-}$ octahedra that provide an octahedral environment for Mn^{4+} upon substitution of Si by Mn.

Na_2SiF_6 is a material with space group symmetry P$\bar{3}$21 (No. 150). The crystallographic unit cell contains three $[SiF_6]^{2-}$ octahedra and six Na^+ ions. There are two crystallographically nonequivalent Si sites in the structure.

In the present work, the structures of perfect and Mn^{4+}-doped Na_2SiF_6 (Mn substituting for Si) were investigated using ab initio calculations within density functional theory (DFT) employing the GGA approximation and the LCAO method, as implemented in the CRYSTAL23 software package. As a result of the calculations, the optimized geometries, electronic, vibrational, dielectric, and elastic properties were obtained. Structural optimization was performed for two spin states (1/2 and 3/2) and two nonequivalent positions of the Mn ion in the crystal lattice. Calculations reveal that the minimum energy corresponds to a total spin of 3/2 for both Mn locations, with three unpaired electrons localized on the Mn ion. The obtained results are discussed and compared in detail.

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Keywords

Phosphor, DFT, LCAO, hexafluorosilicate

Acknowledgements

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Materials for Energy

Measurement of shallow dopants concentrations in polycrystalline silicon by low-temperature FTIR Spectroscopy

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Silicon remains the primary material for microelectronics. This underscores the importance of developing new production technologies and methods for studying its purity and structure.

We have further developed the low-temperature FTIR spectroscopy method to be applicable to measure the Boron, Phosphorous and Aluminum content in polycrystalline silicon for concentrations in the range of ppta. Absorption spectra of polycrystalline silicon samples were measured at 8 K and correlated to the dopant density obtained by four point probe resistivity measurements.

The results of measurements of silicon polycrystals grown by KEPP EU AS using electron beam melting were compared with those of single crystals grown using Float Zone process. The main limitation of using the SEMI/ASTM MF1630-0704 standard when measuring polycrystalline samples is the wide spectral line width and significant scattering [1]. Comparison of the spectra shows that the spectral bands of boron, phosphorus and aluminum in our polycrystalline silicon samples are not significantly wider than the corresponding bands in single crystals. The scattering in our samples is not significantly higher than in samples of single-crystal silicon. It is shown that common calibration factors, derived from a correlation with four-point probe resistivity measurement, can be applied to polycrystal silicon, as well.. It should be noted that such specific properties of silicon polycrystals (allowing the measurement of impurity concentrations by a standard method) are possibly inherent only to polysilicon grown by the electron beam melt growth method. We performed domain structure studies using the polarization properties of the silicon 520 cm^{-1} Raman line. Confocal Raman microscopy was used to create two-dimensional Raman signal intensity maps showing variations in domain orientations.

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Keywords

Silicon, Contaminants, FTIR spectroscopy

Acknowledgements

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Microfluidics and Biomedical technologies

Shear stress in viscoelastic cell media within villus-mimetic gut-on-chip

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Organ-on-a-chip enable dynamic culture conditions that more closely approximate in vivo physiology than conventional static cell cultures [1]. Flow dynamics are known to influence cellular proliferation and differentiation. However the impact of cell-induced features, such as villus-like formations in gut-on-a-chip models, on local flow profiles remains incompletely characterized. [2], [3]

To replicate these structures in a microfluidics system, pillar geometries were derived from endpoint image analysis (n = 3) of a gut-on-chip model. The model consisted of an HT29-MTX and Caco-2 co-culture, cultivated under flow conditions for 8 days. Based on these parameters a device consisting of six different pillar arrays was developed. The pillar diameters ranged from 50 to 140 µm, with centre-to-centre spacing between 165 and 215 µm, while the pillar height was fixed at 70 µm.

The devices were fabricated using an OSTE–COC process. Bulk channel structures were produced from cyclic olefin copolymer (COC) by micromilling, while fine microstructure and device bonding was achieved using off-stoichiometry thiol-ene (OSTE) reaction injection moulding. [4], [5]

Three-dimensional flow fields around the pillar structures were characterized using micro-particle image velocimetry with deionized water and cell culture medium (DMEM + 10% fetal bovine serum). The measurements were compared with three-dimensional COMSOL Multiphysics simulations to determine how villus-like structures affect local flow behaviour and shear stress distributions, providing insight into the physical constraints of villus growth in OOC models.

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Keywords

Organ-on-chip, Particle Image Velocimetry, Fluid shear stress, Microfluidics.

Acknowledgements

This research is funded by the Latvian Council of Science, project “Quantitative Biosensing in Organ-on-Chip Systems” No. LZP-2024/1-0329.

Theoretical Modeling of Functional Materials and Devices

EPR and DFT investigation of neutron-radiation-induced defects in gallium gadolinium garnet

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Gallium gadolinium garnet (GGG) belongs to the garnet crystal family. It has been extensively studied as a laser[1] and scintillator[2] material, but pure GGG is most frequently utilised as a substrate for magnetic thin films. Studying radiation-induced defects is important for materials that are exposed to ionising radiation during normal use, as the accumulation of radiation damage can impact their optical or scintillating properties.

Electron paramagnetic resonance (EPR) spectroscopy was applied to investigate paramagnetic centres in neutron irradiated (E = 1 eV; fluence 10^{20} cm^{-2}) in GGG[3]. The dominant paramagnetic centre is a Ge impurity arising from neutron capture on Ga. By comparing the literature data with density functional theory (DFT) calculations, it is believed that the centre is in $4s^2 4p^1$ (Ge^+) charge state. For such a defect to exist in GGG, Ge would have to be coupled with several oxygen vacancies. On top of that, significant structural changes after neutron irradiation need to have taken place since EPR signals do not represent angular dependences characteristic of cubic symmetry. Other paramagnetic centres present in the material are believed to be some type of rare-earth ion impurity, which cannot be conclusively identified due to the unusual resonance position dependence on temperature. Some form of temperature-dependent magnetic phase transition could explain the EPR signal evolution in GGG[4].

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Keywords

neutron-radiation-induced defects, colour centres, electron spin resonance, gadolinium gallium garnet

Acknowledgements

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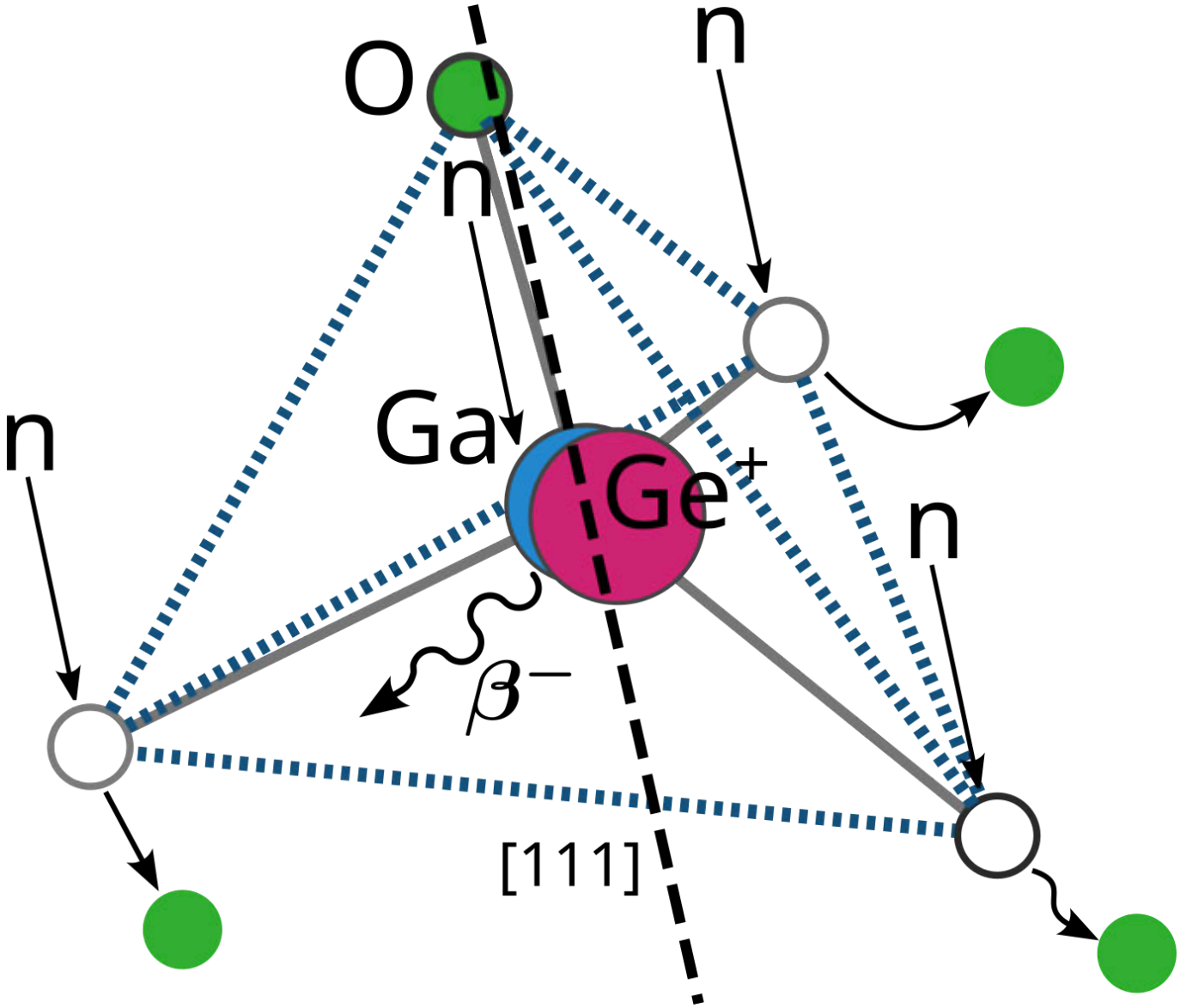

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Guided-Mode Resonance Enabled by Nanosecond Laser-Induced Metasurfaces on Silicon-on-Insulator

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Nanosecond laser processing provides a scalable alternative to ultrafast methods for fabricating functional photonic nanostructures [1,2]. Here, we study laser-induced metasurfaces on silicon-on-insulator (SOI) wafers and their role in structural color generation. Samples were irradiated with 532 nm, 4 ns pulses at 10 Hz on SOI substrates with a 55 nm Si layer and 145 nm buried oxide. Scanning (0.85 mm beam, 0.5 mm/s speed, 0.2 mm hatch) yielded uniform patterning over millimeter scales.

SEM and AFM reveal quasi-periodic gratings (500–600 nm period, ~20 nm depth) decorated with 50–100 nm nanoparticles. Processing in argon suppresses oxidation and improves feature definition. These structures produce green structural color at oblique angles, contrasting with the angle-independent pink of untreated areas.

Angle-resolved reflectance shows a narrow peak near 535 nm, with weak angular dispersion (~30 nm shift from 30°–75°), indicating non-diffraction-dominated behavior. FDTD simulations confirm that the response arises from coupling of diffracted orders (m = −1) with weakly confined waveguide modes [3].

The optical behavior is consistent with guided-mode resonance combined with Fabry–Perot interference. The resonance wavelength scales with Si thickness, enabling tunable colors (e.g., green at 55 nm, red at 70 nm). This demonstrates a maskless route to low-iridescence structural color on SOI for applications such as secure marking and process control.

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Technologies and Devices

Deposition optimization and characterization of structural and anticorrosion properties of HEA thin films obtained via DC Magnetron Sputtering

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High-entropy alloys (HEAs) represent an emerging class of advanced materials distinguished by their structural stability and superior performance in corrosive environments. In this work, HEA-based thin films were fabricated using DC Magnetron Sputtering, with the aim of evaluating the influence of deposition parameters on the microstructure, composition, and anticorrosive performance of the films. The depositions were carried out on silicon and 304L stainless steel substrates, using a hybrid PVD system. The power was varied between 300–500 W and the sputtering time between 25–80 minutes. Morphological and chemical characterization by SEM–EDS revealed the formation of dense, homogeneous films with a well-defined columnar structure for the coatings deposited at 300 and 400 W. The film thickness varied between 1.3 µm and 2.6 µm. The chemical composition of the films was close to the nominal target composition, although more pronounced deviations were observed for Cu, Cr, and Fe at 500 W, where the process became unstable, leading to partial target melting and the formation of porous microstructures.

Scratch tests showed superior cohesion and mechanical stability for the films deposited at 300–400 W, whereas the coatings obtained at 500 W exhibited cracking and reduced adhesion. Electrochemical evaluation in 3.5% NaCl solution demonstrated that the films deposited at 300 W provide the best corrosion resistance, exhibiting the lowest current density and the highest polarization resistance [1]. The results confirm that the optimal power for depositing HEA is 300 W, leading to adherent thin films with superior anticorrosive properties, highlighting the potential of these materials for applications in aggressive environments.

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Keywords

HEA based- thin films, DC Magnetron Sputtering, anticorrosion properties

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Theoretical Modeling of Functional Materials and Devices

Modeling the Direct Current Sputtering Process for High-Entropy Alloys

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The current study presents a comprehensive numerical simulation of direct current cathodic sputtering of a high-entropy alloy consisting of Al, Fe, Cr, Ni, Mn, and Cu using MATLAB [1]. The simulation is carried out by integrating the Yamamura sputtering model with plasma equations under specific conditions of 2.10×10^{-3} mbar pressure, 300 W applied power, a target diameter of 50 mm, and a deposition time of 40 minutes. The results of the simulation show that the three-dimensional spatial distribution of argon ions is non-uniform and reaches a peak of 27×10^{16} m^{-3} at a ring position of 16-17 mm from the center of the magnetron target. The results of the simulation of incident ion flux show a peak of 4.3×10^{20} $m^{-2}s^{-1}$ at a position of 16-17 mm from the center of the magnetron target and dictate the non-uniformity the erosion of the target material. The maximum erosion rate is 7.6 nm s^{-1} at a position of 15-16 mm from the center of the magnetron target and results in a total depth of 18.5 μm after 40 minutes of deposition. The results of sputtering yield calculations of individual elements show that Cu is enriched the most with a sputtering yield of 1.87

atoms/ion compared to Ni (1.74 atoms/ion), Fe (1.49 atoms/ion), Cr and Mn (each having a sputtering yield of 1.38 atoms/ion), and Al having the least sputtering yield of 0.99 atoms/ion. The simulation results are compared with the composition of the material and show that Fe approaches stoichiometric composition (-0.07%), Al is depleted most (-3.36%), and Ni and Cu are enriched most in the material composition (+3.18% and +3.20%, respectively). The material transfer is governed by sputtering yield values of individual elements and provides quantitative results of interest for optimizing composition of targets [2].

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Keywords

cathodic sputtering simulation, Yamamura model, high-entropy alloys, plasma density, target erosion.

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Microfluidics and Biomedical technologies

Scalable manufacturing of a high-shear microfluidic test section for Point-of-Care clotting assessment, CLOTcheck

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Background: Point-of-care (POC) translation of hemodynamic assays demands microfluidics that are physiologically faithful and manufacturable at scale. Shear-induced platelet aggregation (SIPA) is key for arterial thrombosis, yet reproducible high-shear sections are hard to mass-produce.

Objective: To design and manufacturing-validate the CLOTcheck high-shear microfluidic test section (“tip”) for injection molding.

Methods: A multi-channel manifold was redesigned from lab prototypes to an injection-moldable polymer part assembled by ultrasonic welding and followed by surface functionalization. Finite-element flow modeling with Monte-Carlo tolerance analysis defined the allowable geometry window to maintain target wall-shear rates. Quality control used high-precision profilometry for channel dimensions and pressure/flow testing for leakage.

Results: Pilot runs achieved <1% dimensional error. The multi-channel architecture reduced inter-sample and intra-assay variance and enabled stable SIPA-driven occlusion without blow-out artifacts. The end-volume (EV) readout was consistent across batches, correlated with time-to-occlusion (R^2=0.883), and showed <15% intra-device variability.

Conclusions: Manufacturing-led design enables a scalable, injection-molded high-shear sensor that bridges prototyping to clinical POC use, supporting antiplatelet monitoring and trauma diagnostics, developed in Latvia.

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Keywords

Microfluidic Manufacturing, Point-of-Care Diagnostics, Injection Molding, Shear-Induced Platelet Aggregation

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Ferroelectrics and Functional Materials

Na-SUBSTITUTED NdMnO3 PEROVSKITES: SYNTHESIS AND CHARACTERIZATION

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Rare-earth manganite perovskites with the general formula $RMnO_3$ (R – rare-earth element) belong to strongly correlated systems where charge, spin, orbital, and lattice interactions are closely coupled. In these compounds, the distortion of MnO_6 octahedra, governed by the ionic radius of the A-site cation and the tolerance factor, determines structural stability and physical properties. Owing to their potential in multiferroic and magnetoelectric applications, rare-earth manganites attract significant attention, as structural distortions and spin–lattice coupling may induce coupled magnetic and electric responses.

$NdMnO_3$ is of particular interest due to the interaction between Mn and Nd magnetic sublattices, leading to complex magnetic ordering and sensitivity to structural modifications. Chemical substitution at the A-site represents an effective strategy for tuning its properties. Partial replacement of Nd^{3+} with Na^{+} alters the Mn^{3+}/Mn^{4+} ratio through charge compensation, affecting magnetic ordering and phase stability. However, studies have mainly focused on low Na concentrations, while the effect over a wider compositional range remains insufficiently explored.

In this work, $Nd_{1-x}Na_xMnO_3$ (x = 0–0.6) samples were synthesized by the sol–gel method using ethylene glycol as a complexing agent to ensure homogeneous cation distribution. Phase formation and crystal structure were analyzed by XRD and FT-IR spectroscopy, while morphology and composition were examined by SEM, SEM–EDX, and ICP–OES. The results confirm successful synthesis and reveal the influence of A-site substitution on structural and compositional characteristics.

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Keywords

sol-gel, perovskites, manganite

Materials for Photonics

Microwave-assisted synthesis of doped zinc sulfide electroluminescent phosphors

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Doped zinc sulphide (ZnS) materials exhibit excellent optical and electrical properties, making them superior materials for photoluminescent (PL) and electroluminescent (EL) devices. This study focuses on demonstrating the possibility of synthesizing ZnS doped with various transition and rare-earth elements (ZnS:Mn; ZnS:Cu,Cl; ZnS:Nd; ZnS:Ag,Co) for further application in the fabrication of Alternating Current Thick-Film Electroluminescent (ACTFEL) devices using microwave-assisted (MW-assisted) solvothermal and hydrothermal methods. The main advantages of microwave-assisted chemical processes are the increased reaction rate and yield, as well as uniform mixture heating, which leads to the formation of particles with a narrow size distribution and high crystallinity. This method is known as one of the most innovative green chemistry synthesis methods.

This study demonstrates how MW-assisted synthesis enables the incorporation of different dopants into ZnS materials. The incorporation of dopant ions from the reaction mixture into the crystalline structure of the synthesized materials was evaluated by energy-dispersive X-ray analysis. The amount of incorporated dopant for each material was then compared to the integral EL intensity. For the assessment of EL intensity, ACEL devices were fabricated by the procedurepreviously described by Klave et al. [1]

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Keywords

microwave synthesis, zinc sulfide, electroluminescence

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Materials for Energy, Large-Scale Research Infrastructures, Science Policy and Collaboration

X-ray absorption spectroscopy studies of protonation-induced electronic and structural changes in WO_3 nanoparticles

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Tungsten(VI) oxide (WO_3) is a widely studied material for solar panel applications owing to its photochromic properties [1]. The reversible color switching observed in WO_3 originates from changes in its electronic structure and local atomic arrangement [1]. As a result, X-ray absorption spectroscopy is a suitable technique for studying these processes.

WO_3 nanoparticles (NPs) were prepared via the polyol synthesis route [2]. X-ray diffraction analysis showed an average NP grain size of about 3 nm. Protonated WO_3 NPs were obtained through hydrogen spillover on metallic indium in an acidic environment.

X-ray absorption spectroscopy at the W L_3-edge was performed at 300 K at the DESY PETRA III P64 and P65 beamlines (Hamburg, Germany) [3,4]. High-energy-resolution fluorescence-detected X-ray absorption near-edge structure (HERFD-XANES) and extended X-ray absorption fine structure (EXAFS) spectra were collected for both protonated and non-protonated samples. EXAFS spectra were analyzed using the Reverse Monte Carlo (RMC) method enhanced with an evolutionary algorithm [5].

HERFD- XANES analysis suggests preferentially octahedral coordination of tungsten ions in NPs. RMC modeling of the EXAFS spectra indicates that the protonation leads to a displacement of tungsten atoms toward the center of the octahedra, and the WO_6 octahedra become less distorted.

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Keywords

Tungsten (VI) oxide, HERFD-XANES, EXAFS, Reverse Monte Carlo

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Ferroelectrics and Functional Materials, Technologies and Devices

Preparation and characterisation of GaN-Al2O3-NbSe2 core-shell nanowires

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In this work, the growth of GaN-Al_2O_3-$NbSe_2$ core-shell nanowires (NWs) was successfully demonstrated. As a well-known superconductor, $NbSe_2$ in a shell configuration on NWs can offer a promising platform for investigating its properties at reduced dimensions.

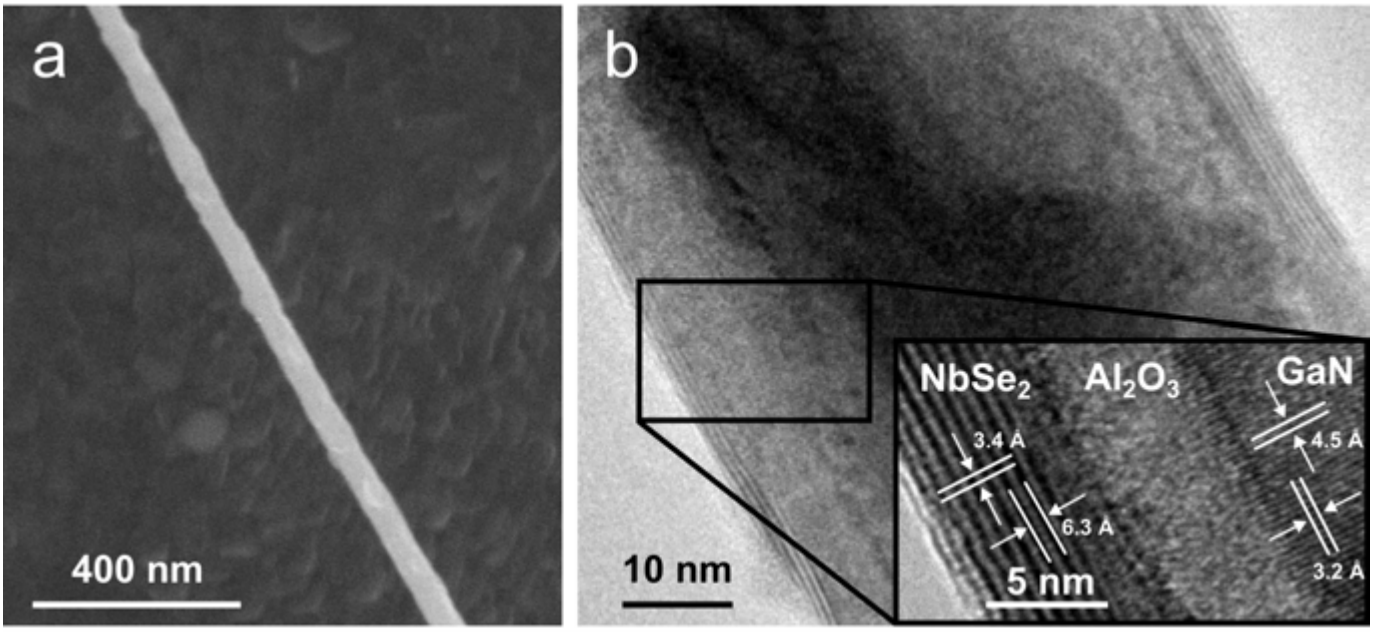
GaN NWs were fabricated via the vapour-liquid-solid (VLS) growth, and an amorphous Al_2O_3 interlayer was obtained by atomic layer deposition (ALD) to provide the NW surface passivation. The $NbSe_2$ shell was formed through a two-step process involving magnetron sputter deposition of a Nb layer onto the GaN-Al_2O_3 NWs followed by a selenization process in a chemical vapour deposition (CVD) reactor. The process parameters were optimised to achieve uniform and crystalline shell formation while preserving the NW morphology.

The resulting nanostructures were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy, confirming the successful formation of GaN-Al2O3-NbSe2 core-shell NWs and providing insight into their morphology, crystal structure, and chemical composition.

Figure 1. (a) SEM and (b) TEM images showing the morphology and structure of the as-grown GaN-Al_2O_3-$NbSe_2$ core-shell NWs

Keywords

core-shell nanowires, niobium diselenide, superconductor


a
400 nm
b
10 nm
NbSe2
Al2O3
GaN
3.4 Å
6.3 Å
4.5 Å
3.2 Å
5 nm

Materials for Photonics

Influence of Sapphire Substrate Orientation on Epitaxial Rutile GeO_2 Thin Film Solar-Blind Photodetector Properties

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Rutile GeO_2 (r-GeO_2) has recently emerged as a promising ultrawide-bandgap (E_g~4.7 eV) semiconductor due to its potential use as a solar-blind UV-C range photodetector and its theoretically predicted ambipolar doping, which implies unique device fabrication possibilities. However, producing phase pure r-GeO_2 still remains challenging due to many unknown variables both in substrates and deposition methods [1]. In this work, pulsed laser deposition process for r-GeO_2 thin film growth on a-, m- and r-plane sapphire substrates was demonstrated in 350 – 425 °C temperature range, and film crystallinity and morphology optimization was performed. X-ray diffraction (XRD), X-ray photoelectron spectroscopy, scanning and transmission electron microscopies, atomic force microscopy (AFM), Raman spectroscopy and ellipsometry were used for the as-grown film characterization. XRD analysis revealed that (101)-orientated r-GeO_2 films were obtained on a- and r-plane sapphire substrates, while (002) orientation for m-plane substrate was observed. At optimized deposition conditions for each substrate orientation, XRD omega scan peak full width at half maximum and AFM surface roughness scan yielded results of 0.66°/5.1 nm, 0.5°/2.7 nm and 1.2°/6.9 nm for a-, m- and r-plane substrates, respectively. Furthermore, photodetector devices fabricated on these films exhibited peak responsivities 1.76 mA/W, 1600 mA/W and 5.77 mA/W for a-, m- and r-plane substrates, accordingly. It was observed that the responsivity peak wavelength at 220-230 nm for all the prepared films corresponds to a value significantly larger than the optical bandgap, which merits to be investigated further.

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Keywords

Germanium oxide, thin film, photodetector

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Materials for Photonics

Characterisation of Fabry-Pérot resonators fabricated via grayscale UV lithography and their application to the investigation of strongly coupled systems

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The research of strongly coupled systems is of great importance due to their high potential for practical applications, which are expected to lead to new technological advancements in optics and photophysics, photochemistry, quantum mechanics, polaritonic chemistry, hydrogen technologies, as well as in the study and utilisation of room-temperature Bose-Einstein condensation[1–6].

The main objective of this work was to investigate polaritonic states arising in strongly coupled systems in Fabry-Pérot resonators, which were fabricated via grayscale UV lithography using a back focal plane spectrometer based on the Olympus BX51 microscope[7]. The optical properties of resonators fabricated via grayscale UV lithography were analysed in parallel[8,9]. An important advantage of grayscale lithography is that it produces multiple resonators with different thicknesses within a single fabrication cycle. This significantly increases efficiency and flexibility compared to traditional fabrication methods.

Based on these results, a deeper understanding of Fabry-Pérot resonators designed to study strongly coupled systems can be achieved. This research demonstrates that grayscale UV lithography is highly suitable for fabricating high-quality optical cavities and contributes more broadly to exploring light-matter interactions, paving the way for novel photonic structures and applications.

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Keywords

Fabry-Pérot resonators, strong coupling, grayscale UV lithography

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Early-Stage Development of Eco-Friendly NIR Persistent Phosphors for Remote Forest Monitoring

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Near-infrared (NIR) persistent luminescent materials enable passive optical detection under low-light conditions and are promising for non-invasive environmental monitoring. However, most known NIR persistent phosphors require UV or X-ray excitation, limiting their applicability in real-life situations. In this work, we report on the early-stage development of eco-friendly, sunlight-activated persistent luminescent materials based on Cr^{3+}-activated perovskite-type hosts. Selected $MTiO_3$ (M = Mg, Ca, Sr, Ba) compositions were synthesised and investigated using photoluminescence and thermally stimulated luminescence spectroscopy to evaluate emission characteristics and charge trapping processes. Initial material screening indicates near-infrared emission and persistent luminescence following optical excitation, demonstrating the potential of Cr^{3+}-activated perovskites as environmentally benign NIR persistent phosphors. Ongoing work focuses on defect-related mechanisms and optimisation of composition to enhance emission persistence. The presented results establish a foundation for the development of sustainable optical materials for remote monitoring applications.

Keywords

persistent luminescence, perovskite, near-infrared radiation, forest monitoring, optical materials

Acknowledgements

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Materials for Energy

Ab initio calculations of the high voltage 5 Volt rechargeable Li ion battery cathode Li2CoMn3O8 and new battery anodes

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Nowadays, Li-ion batteries are the state-of-the-art power sources operating mainly in the 4 Volt regime. Ab initio calculation results by means of the FP-LAPW method, using the computer code WIEN2k, for battery cathode material $Li_2Co_xMn_{4-x}O_8$ (x = 0, 1, 2, 3, and 4) are presented [1-3]. The ab initio computed average battery voltage for $Li_2CoMn_3O_8$ cathode material is around 5 Volt [1-3]. The ab initio computation result for a 5 Volt average battery voltage excellently describes recently experimentally synthesized $LiCo_{0.5}Mn_{1.5}O_4$ battery cathode material, which exhibited a discharge plateau starting at around the 5 Volt. The ab initio computed average battery voltages for other x values in the cathode material $Li_2Co_xMn_{4-x}O_8$ (x = 0, 2, 3, and 4) are equal to (3.95V; 4.47V; 4.19V, and 3.99V, respectively) [1-3].

The monolayer carbon allotrope, Me-graphene (called also C_{568}), was respectively doped with Al, Si, P, and Ge atoms by substituting the sp^3-hybridized carbon atom in its unit cell to manipulate its physical properties [4]. Ab initio computations using the density functional theory (DFT) confirmed the dynamic stabilities of the related doping systems. According to ab initio HSE06 computations, after doping with Si atom, the band gap of the Me-graphene system decreased from 1.097 eV to 0.987 eV [4]. Nevertheless, the Ge-dopant at the sp^3-site has very limited influence on the band gap. Whereas with Al and P dopants, the systems changed to be metallic because their Fermi levels cut into the valence bands. In addition, the adsorption sites of Li atoms and the energy profiles of the Li migrations on the related 2D material systems were also investigated in order to reveal their application potentials as anodes in lithium ion batteries [4].

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Keywords

Li-ion battery, new cathode material, new anode material, 5 Volt rechargeable Li-ion battery

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Technologies and Devices

Lossy Mode Resonance Sensor Based on Indium Tin Oxide and Polyaniline Thin Films for Ammonia Detection

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Ammonia monitoring is important for improving environmental conditions in livestock farming, industrial safety, and air quality control. However, conventional ammonia sensors often suffer from limited operational lifetimes and poor selectivity due to the chemically aggressive nature of ammonia and interference from environmental factors. In this work, we focus on the development of a photonic sensing approach based on the lossy mode resonance (LMR) phenomenon using a planar glass waveguide platform. The proposed sensing structure consists of a glass waveguide coated with a lossy indium tin oxide (ITO) layer for LMR excitation and a polyaniline (PANI) functional layer intended for selective interaction with ammonia molecules. The ITO thin film is deposited by magnetron sputtering, while the PANI layer is grown on top of the ITO coating via electrochemical polymerization. Numerical simulations are performed to optimize the thickness and optical properties of the coatings in order to achieve resonance at the desired operating wavelength. Alongside the sensing structure, a complete experimental prototype is developed, comprising an optical excitation and detection system with a light source, spectrometer, and optical components required for efficient coupling of light into the waveguide. The fabricated structures and deposited films are characterized using ellipsometry, optical microscopy, and scanning electron microscopy to determine the thicknesses of the coatings and evaluate the homogeneity of the deposited layers through cross-sectional inspection of the device. Optical measurements are performed to confirm the excitation of LMR and to evaluate the spectral response and stability of the developed structures. The presented work contributes to the advancement of LMR-based photonic sensing techniques and provides a foundation for future gas sensing applications, including ammonia detection.

Keywords

amonia, lossy mode resonance, sensors

Acknowledgements

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Microfluidics and Biomedical technologies

GENetic EXtraction device for next generation DNA extraction

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Genomics has become central discipline in modern biology, medicine, and biotechnology, enabling applications ranging from precision medicine to population-scale sequencing [1,2]. The quality and reliability of genomic analysis strongly depend on upstream sample preparation, particularly DNA extraction, which remains a key bottleneck in many sequencing workflows [3,4]. Conventional extraction methods often rely on chemical purification or filter-based separation technologies that introduce process variability, require multiple manual handling steps, and are difficult to integrate into automated or miniaturized systems [3].

Herein we propose GENEX – an electrode-based DNA extraction technology designed for rapid and reproducible nucleic acid isolation with a focus on ease of integration within existing laboratory workflows. The platform employs a patented precision engineered 3D electrode, which enables electrostatic capture and controlled release of DNA molecules.

GENEX system shows non-inhibitory behavior towards PCR amplification, ensuring compatibility with downstream molecular biology analysis and workflows. Initial validation experiments demonstrate successful DNA extraction from buffer samples, with minimal nonspecific adsorption to the electrode surface, and preserved sample compatibility with PCR-based analysis.

These results demonstrate the feasibility of the GENEX concept as a scalable DNA extraction module capable of simplifying sample preparation and facilitating integration into future sequencing and molecular diagnostic workflows.

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Keywords

DNA extraction, sample preparation, electrostatic surfaces

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Microfluidics and Biomedical technologies

Influence of glucose oxidase immobilization technique on electrochemical glucose sensor performance

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Organ-on-chip systems require reliable methods for monitoring metabolic activity in real time, with glucose serving as one of the most important biochemical indicators of cellular metabolism[1]. Electrochemical glucose sensors based on glucose oxidase (GOx) are widely used due to their sensitivity and ability to measure glucose continuously in real time[2]. However, the sensor performance strongly depends on the enzyme immobilization strategy, influencing enzyme loading, catalytic activity, and electron transfer at the electrode interface[3]. Understanding how different functionalization approaches influence these properties is therefore essential for the development of robust bioelectrochemical interfaces.

In this work, the influence of three GOx immobilization strategies on electrochemical glucose sensing was investigated. The methods included physical adsorption, linker-based immobilization, and enzyme copolymerization. Enzyme loading and catalytic activity were evaluated using a spectrophotometric assay, while electrochemical performance was characterized by cyclic voltammetry to determine sensitivity and limit of detection.

Among the approaches investigated, glucose oxidase copolymerization provided the highest catalytic activity with the lowest variability between samples, resulting in the lowest limit of detection and highest specificity. This highlights the importance of enzyme immobilization strategy in defining the performance of real time glucose sensors and provides insight into the design of bioelectrochemical interfaces relevant for organ-on-chip monitoring.

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Keywords

Glucose sensing, electrochemical sensors, immobilization

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Materials for Energy, Materials for Photonics

Characterization of neutron induced defects in Al_2O_3 ceramics using optical absorption, TSL, and Raman methods

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Al_2O_3 ceramics are widely used in nuclear and fusion environments due to their high stability and wide bandgap. This study examines pure undoped, sintered, vanadium-doped, nickel-doped, and rare-earth–activated ceramics irradiated with neutron fluences of 10^{21}, 10^{22}, and 10^{23} n/m².

Optical absorption measurements reveal characteristic defect centers, including F centers at ~6 eV and F^+ centers near ~5 eV. Aggregated vacancy defects such as F_2, F_2^+, and F_2^{2+} are also observed in the visible range. Dopant-related features, including V^{3+}/V^{4+} charge-transfer bands and Ti^{3+} absorption, further modify the spectra. These results indicate that neutron irradiation generates oxygen vacancies, alters their charge states, and promotes defect clustering.

Thermally stimulated luminescence (TSL) measurements show complex glow curves containing 4–7 trapping levels. Most trap energies fall within 0.5–1.3 eV, while deeper traps up to ~3 eV contribute to long-term charge storage. Undoped samples exhibit trap energies from 0.51 to 2.86 eV, whereas vanadium-doped ceramics show pronounced deep traps around 2 eV. All compositions display a similar defect structure dominated by oxygen-vacancy–related centers. Vanadium enhances high-temperature luminescence by stabilizing deep traps, while nickel reduces luminescence efficiency by acting as a non-radiative recombination center.

Raman spectroscopy indicates irradiation-induced lattice strain consistent with vacancy formation and aggregation.

Overall, the results demonstrate that neutron fluence and impurities govern trap distribution and recombination pathways. These findings confirm that Al_2O_3 ceramics remain strong candidates for radiation-dosimetry and sensing applications in high-flux neutron environments.

Keywords

Al_2O_3 ceramics; neutron irradiation; optical absorption; thermally stimulated luminescence (TSL); trap levels; Raman spectroscopy; radiation dosimetry.

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Materials for Energy

ELECTROCHEMICAL PERFORMANCE OF CARBON NANOTUBES IN AQUEOUS ZINC ION BATTERIES

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Electrode materials incorporated with carbon nanotubes (CNTs) exhibit advanced electrochemical performance in aqueous zinc-ion batteries (AZIBs) due to high surface area and more efficient Zn^{2+} ion transport pathways, which together improve cycling stability. [1,2]. Usually, CNTs are considered as an additive that improves the electrical conductivity of the electrode. Only Y. Tian with co-authors discussed the properties of multi-walled CNT (MWCNT) electrodes in zinc-ion capacitors [3], however the role of bare CNTs in AZIBs has not been thoroughly investigated yet.

In this work, networks of single-walled (SWCNTs) and MWCNTs were tested as cathodes in AZIBs. The networks were fabricated via spray-coating deposition for SWCNTs and drop-coating deposition for MWCNTs, respectively. Structural characterization of prepared cathodes was carried out using scanning electron microscopy (SEM), while electrochemical performance was evaluated through galvanostatic charge-discharge (GCD), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques.

Electrochemical measurements of different CNT cathodes revealed that they have stable cycling performance, but specific capacities values are lower in comparison with other electrodes studied. Nevertheless, participation of CNTs in electrochemical processes must be taken into consideration when creating composite electrodes for AZIBs.

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Keywords

aqueous zinc ion batteries, carbon nanotubes, cathode

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The research was supported by the project «Application of Bi2Se3-CNT heterostructures for conventional and photo-assisted low temperature rechargeable Zn-ion batteries» (project No. lzp-2024/1-0187).

Materials for Energy

ELECTROCHEMICAL PERFORMANCE OF CARBON NANOTUBES IN AQUEOUS ZINC ION BATTERIES

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Electrode materials incorporated with carbon nanotubes (CNTs) exhibit advanced electrochemical performance in aqueous zinc-ion batteries (AZIBs) due to high surface area and more efficient Zn^{2+} ion transport pathways, which together improve cycling stability [1,2]. Usually, CNTs are considered as an additive that improves the electrical conductivity of the electrode. Only Y. Tian with co-authors discussed the properties of different multi-walled CNT (MWCNT) electrodes in zinc-ion capacitors [3], however the role of single-walled CNTs (SWCNTs) in AZIBs has not been thoroughly investigated yet.

In this work, networks of SWCNTs and MWCNTs were tested as cathodes in AZIBs and properties of SWCNTs were investigated and compared with MWCNTs. The networks were fabricated via spray-coating deposition for SWCNTs and drop-coating deposition for MWCNTs, respectively. Structural characterization of prepared cathodes was carried out using scanning electron microscopy (SEM), while electrochemical performance was evaluated through galvanostatic charge-discharge (GCD), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) techniques.

Electrochemical measurements of different CNT cathodes revealed that they have stable cycling performance, but specific capacities values are lower in comparison with other electrodes studied. Nevertheless, participation of CNTs in electrochemical processes must be taken into consideration when creating composite electrodes for AZIBs.

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Keywords

aqueous zinc ion batteries, carbon nanotubes, cathode

Acknowledgements

The research was supported by the project «Application of Bi2Se3-CNT heterostructures for conventional and photo-assisted low temperature rechargeable Zn-ion batteries» (project No. lzp-2024/1-0187).

Materials for Energy

Solvothermal Synthesis of Bismuth Selenide and Single-Walled Carbon Nanotube Heterostructures for Improved Charge Storage in Aqueous Zinc-Ion Batteries

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Understanding and improving ion and electron transport in cathode materials remains a key challenge for aqueous zinc-ion batteries (AZIBs), where sluggish Zn^{2+} diffusion, limited electronic conductivity and structural degradation restrict performance [1]. Designing heterostructured cathodes that combine efficient ion diffusion with enhanced electron transport is a promising approach to address these challenges.

Bismuth selenide (Bi_2Se_3), a layered material with a van der Waals structure, is a promising cathode for AZIBs, as it enables Zn^{2+} intercalation between weakly bonded layers [2]. Incorporation of single-walled carbon nanotubes (SWCNTs) improves electrical connectivity by forming a conductive network and can enhance mechanical stability during cycling. In Bi_2Se_3/SWCNT heterostructures, interfacial interactions facilitate ion and electron transport, while local electric fields associated with possible p-n junctions may promote charge transfer.

Bi_2Se_3/SWCNT heterostructures with different Bi_2Se_3:SWCNT ratios were synthesized via a solvothermal method to evaluate the effect of composition on electrochemical performance. Structural and compositional properties were analyzed using scanning electron microscopy and atomic force microscopy. Electrochemical performance was studied by cyclic voltammetry and galvanostatic charge-discharge measurements, demonstrating improved charge storage behavior as cathodes for AZIBs.

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Keywords

Zinc-ion batteries, bismuth selenide, single-walled carbon nanotubes, cathode composite materials, solvothermal synthesis

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Materials for Energy, Technologies and Devices

Advanced flexible thermoelectric generator based on carbon nanotubes – inorganic semiconductor heterostructures

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Wearable sensing technology rapidly became an irreplaceable part of daily life. Wearable sensors are flexible, cost-effective, and highly sensitive, which makes them a favorable candidate for future sensing technology. However, for proper operation all these sensors require an external power and rely on batteries, thus having limitations on lifetime and requirement for periodic recharging or replacement of the battery or the device itself. A promising alternative to the conventional batteries is thermoelectric generators able to directly convert thermal energy to electrical.

In this work, a flexible thermoelectric generator (FTEG) employing innovative architecture allowing to effectively convert heat generated by the human's body to the electrical energy is presented. The FTEG is based on ultrathin bismuth and antimony chalcogenide nanostructures deposited directly on prefabricated carbon nanotube (CNT) networks, and the resulting chalcogenide-CNT heterostructures are preserved and protected from the surrounding environment by encapsulation in non-conductive environmentally-friendly, biocompatible, low-cost, and widely available polymer [1].

An innovative deposition technique, allowing deposition of multiple connected in series p-n pairs of thermoelectric elements and advanced element arrangement tolerant to bending and stretching are discussed. The performance of FTEG is characterized at room temperature using temperature differences of 5-30 degrees and different external loads.

The results prove the perspective applications of the presented FTEG for powering microelectronic devices and conversion of domestic heat to valuable electricity.

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Keywords

flexible thermoelectric generator; heterostructures; encapsulation; bismuth and antimony chalcogenides; carbon nanotubes

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Materials for Energy

Hydrogen Generation from Heterogeneous Aluminium Waste by Alkaline Hydrolysis

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Sustainable hydrogen production and efficient waste valorisation are closely linked challenges in the transition toward circular energy systems. Aluminium-water reactions are increasingly recognized as a promising route for on-demand hydrogen generation, and recent reviews highlight their relevance for recycled and scrap-derived aluminium [1,2].

In this work, hydrogen generation by alkaline hydrolysis of heterogeneous aluminium-containing waste is investigated using industrial shavings, laminated packaging, electrical wires, and other composite residues. The results show that hydrogen evolution depends not only on aluminum content, but also on the accessibility of the metallic phase to the alkaline medium. Materials with high exposed aluminum surface area exhibit rapid hydrogen release, whereas laminated and coated wastes react more slowly and less completely because non-metallic barriers restrict solution access. Increased NaOH concentration improves conversion efficiency and reduces passivation, in agreement with trends reported for industrial aluminium scrap hydrolysis [3].

XRD, EDX, and XRF analyses further indicate selective aluminium conversion, while impurity elements remain concentrated in the solid residue. This creates an opportunity to combine hydrogen production with subsequent recovery of secondary metals by hydrometallurgical treatment. The findings support the development of integrated waste-to-hydrogen technologies.

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Keywords

hydrogen production, aluminium waste, alkaline hydrolysis, recycling, circular economy

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Materials for Photonics, Large-Scale Research Infrastructures, Science Policy and Collaboration

Electronic structure and luminescence properties of Rb2GeF6 for application in advanced scintillation technologies

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Rb_2GeF_6 is a wide bandgap material promising for scintillators based on intrinsic emission, yet its fundamental electronic properties and relaxation pathways of electronic excitations remain largely unexplored [1]. The AFLOW database [2] provides information on its electronic band structure, featuring the bottom of the conduction band composed of Rb states and a complex valence band formed by the F, Ge and Rb states hybridized like in other ternary fluorides [3]. A rich electronic structure implies several emission channels, including intrinsic self-trapped excitons (STEs), intra-band and cross luminescence [3]. The experimental research of this material was carried out in the excitation energy range 4.6-45 eV at MAX IV (FinEstBeAMS beamline) in Lund and 3.7-40 eV DESY (P66 beamline) in Hamburg. Cathodoluminescence studies were performed using 10 keV electron beam in Tartu. The emission spectrum of Rb_2GeF_6 covers the UV to visible range with the broad emission bands peaking at 260, 370 and 610 nm at 7 K (Fig. 1). The 370 and 610 nm emissions show excitation bands in the energy gap, thus implying an extrinsic nature of the emission centers. The UV emission showing the onset of its excitation spectrum at 11.2 eV near the fundamental absorption edge is tentatively assigned to STEs. These data allow introducing a scissor factor of ~2 eV to the bandgap value predicted by AFLOW. In the present work, energy relaxation processes and the origin of emissions will be discussed.

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Keywords

Self-trapped excitons, Ternary fluorides, Wide bandgap

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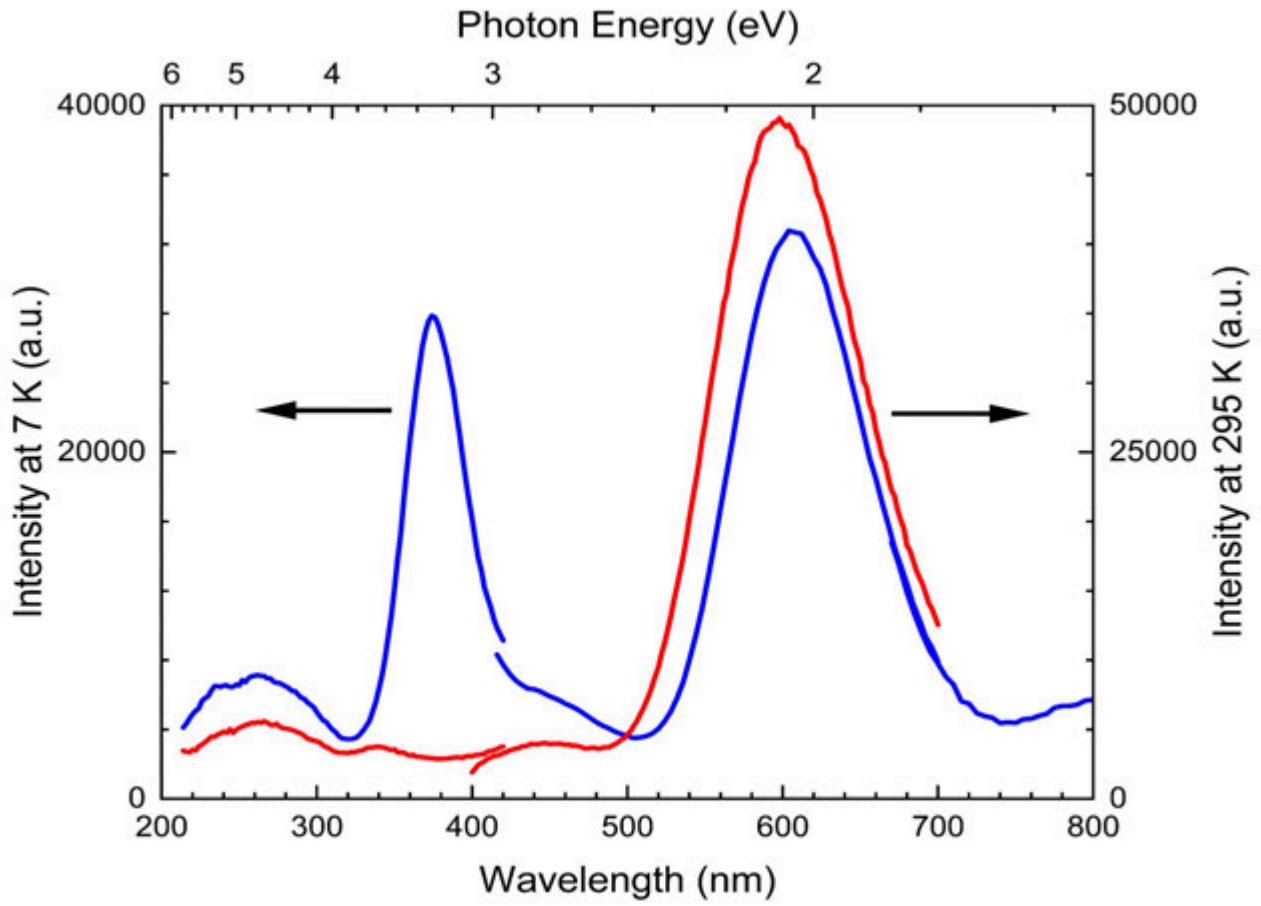

Figure 1: The emission spectra of Rb_2GeF_6 excited by 45 eV photons at 295 (red line) and 7 K (blue line).

Materials for Energy

Alder-based electrodes for supercapacitors

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Supercapacitor is an electrochemical energy storage device that is used in multiple applications where high-power density or rapid charge–discharge capability is demanded. A long cycle life is another advantage of the supercapacitors, but low energy density remains the main limiting issue. An electric double-layer capacitor (EDLC) is a type of supercapacitors that is based on processes in an electric double layer on the surface of an electrode. Typical electrode materials for EDLC include different porous carbon structures like graphite, graphene, carbon nanotubes and others with bio-derived carbons being currently one of the trends in the field [1].

Alder is well-known and widely used wood, e.g., in carpentry due to its mechanical and visual properties. It also is fast growing tree allowing to restock timely. Waste produced during processing (bark, branches etc.) is used for food smoking, charcoal production and many other implementations. In this work properties of alder-based activated carbon materials for aqueous EDLCs electrodes are investigated. We are using carbon made of (1) alder wood [2]; (2) alder wood modified with kraft black liquor and (3) alder bark to determine the best candidate for electrode material.

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Keywords

Energy storage, supercapacitors, EDLC, bio-derived carbon

Acknowledgements

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Theoretical Modeling of Functional Materials and Devices

From DFT to ML for modeling of functional catalyst materials

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Theoretical modeling and artificial intelligence are becoming central tools for predicting next-generation functional materials. The main challenge is to balance computational cost and predictive reliability: Large-scale screening requires evaluating thousands of candidates, while accurate quantum-chemical methods remain computationally demanding. Therefore, workflows that combine density functional theory (DFT), density functional tight-binding (DFTB), and various machine-learning (ML) approaches are becoming increasingly important.

In this work, we discuss atomistic modeling of catalyst–electrolyte interfaces relevant to electrocatalytic reactions. We investigated several ML approaches on standard catalyst materials (see Figure), including the Universal Model for Atoms (UMA), SpookyNet, the Message Passing Atomic Cluster Expansion (MACE), and others, see Ref. 1 and references within. These approaches enable geometry optimization and molecular dynamics simulations of functional materials much faster than conventional DFT calculations.

We then tested the most promising methodologies for the discovery of novel dual-atom-site catalyst materials, extending the workflow from DFT calculations for hundreds of materials to DFTB and ML simulations for thousands. The resulting correction scheme is applied to high-throughput screening of materials from a database containing more than 44,000 potential catalysts, see Ref. 2. The target descriptors include predicted overpotentials, adsorption energies of H- and CO-intermediates related to selectivity, and formation energies under acidic conditions related to stability.

The work shows how ML-assisted computational workflows can accelerate the discovery of functional materials while balancing efficiency and predictive accuracy.

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Keywords

Density Functional Theory, Machine Learning, Dual-atom site catalysts

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Technologies and Devices

Electroluminescent Performance of OLEDs with Ag Nanoparticle-Modified PEDOT:PSS Layer

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This work presents the electroluminescent performance of organic light-emitting devices (OLEDs) containing silver nanoparticles (AgNPs). Spherical AgNPs were synthesized by photoinduced reduction of silver ions with $AgNO_3$ in the presence of trisodium citrate at room temperature. For efficient AgNP-based OLEDs, the localized surface plasmon resonance (LSPR) position should match the emission spectrum of the organic semiconductor.

Two device architectures were fabricated based on electrochemical and photophysical characterization of dimethoxy/difluorobenzothiadiazole core materials:: Device A – ITO/PEDOT:PSS/PVK/PVK:EML/BCP/Ca/Al and Device B – ITO/PEDOT:PSS/AgNP/PVK/PVK:EML/BCP/Ca/Al. The devices were fabricated by combining thermal vacuum deposition with spin-coating techniques. Both devices exhibited electroluminescence spectra consistent with the photoluminescence of the red emissive layer. The turn-on voltage was around 3 V. Device A achieved a brightness of 8500 cd m^{-2} at 382 mA cm^{-2}, while device B achieved 5400 cd m^{-2} at 213 mA cm^{-2} with a quantum efficiency of 4.0%. The incorporation of AgNPs reduces the current density and slightly improves the quantum efficiency,

probably due to the modification of the Fermi level of PEDOT:PSS. Numerical simulations using Setfos show good agreement with the experimental results, confirming the proposed device model.

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Keywords

OLED, Ag nanoparticles, thermal vacuum deposition, Setfos,

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Ferroelectrics and Functional Materials

Simultaneous in situ dielectric and crystallographic temperature dependent measurements

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The dielectric and crystallographic measurements of various materials using X-ray diffraction methods, accompanied by an LCR meter, can be of great use for studying and modifying these materials. Performing these measurements independently can produce larger errors or lead to false conclusions.

In this work, the electrical infrastructure and software needed for these measurements were developed to obtain the XRD pattern and capacitance of materials under varying temperatures simultaneously. From the capacitance data, it is possible to gain information on other properties of the material, such as its dielectric constant.

The system was tested on barium titanate, which has been extensively studied. This ceramic was chosen for its multiple structural phase transitions at different temperatures. The results are well aligned with prior research indicating to the effectiveness of the system.

Acknowledgments: New generation of piezoelectric materials for active vibration control (LZP-2023/1-0571)

Keywords

X-ray diffraction, dielectric permittivity, barium titanate, image processing, simultaneous in situ measurements

Acknowledgements

New generation of piezoelectric materials for active vibration control (LZP-2023/1-0571)

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NEW FLUORENE DERIVATIVES AS EMITTERS AND HOLE-TRANSPORTING MATERIALS BLUE EMITTING OLEDs

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Organic light-emitting diodes (OLEDs) are increasingly used in display and lighting technologies due to their fast response, wide viewing angle, high color quality, and compatibility with flexible devices [1]. However, the development of efficient and stable blue-emitting OLED materials remains a significant challenge because high-energy excitations accelerate degradation processes in organic semiconductors [2]. Another important issue is the fabrication of efficient solution-processed OLEDs, which often show inferior performance compared to devices prepared by vacuum deposition [3]. Next-generation optical communication technologies require OLEDs with very short emission lifetimes enabling high-speed operation [4].

In this work, new fluorene-based organic semiconductors designed for deep-blue emission and efficient hole transport are presented. The synthesis and properties of four compounds containing dimethylfluorene or spirobifluorene cores combined with phenyldibenzofuran or phenylcarbazole peripheral groups are reported. These structural motifs are known to enhance charge transport, thermal stability, and the HOMO–LUMO energy gap required for blue emission [5]. The synthesized materials exhibit deep-blue photoluminescence and short fluorescence lifetimes suitable for high-speed OLEDs. Solution-processed doping-free OLEDs with one synthesized compound as emitter shows deep-blue electroluminescence with CIEx,y coordinates of (0.146, 0.082) and a maximum external quantum efficiency (EQE) of 1.9%. In addition, the spirobifluorene–carbazole derivative demonstrates efficient hole transport and competitive performance in sky-blue thermally-activated-delayed-fluorescence OLEDs, achieving EQE up to 15.8% at 5000 cd m^{-2}.

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Acknowledgements

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Materials for Energy

Structure–Driven Electrochemical Behavior of NaOH-Activated Birch Carbons for Energy Storage

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Birch wood residues were used to produce a series of porous carbons whose structural features were tuned through variations in activation temperature and alkali ratio. The resulting materials exhibited specific surface areas exceeding 2000 $m^2 g^{-1}$ and a transition from predominantly microporous frameworks at 700 °C to mixed micro–mesoporous architectures at 800 °C. Comprehensive characterization (N_2 sorption, Raman spectroscopy, XRD, SEM, XPS) revealed that higher temperatures promote partial graphitization, whereas lower temperatures preserve a micropore-dominated structure with greater accessible surface area. Electrochemical evaluation in symmetric aqueous coin cells showed that the microporous materials provided the highest capacitance, signifficantly surpassing a commercial activated carbon under identical conditions. Although carbons activated at 800 °C displayed more ordered graphitic domains and competitive rate capability, their reduced microporosity limited overall charge storage. These results demonstrate that birch-derived carbons can deliver high performance in aqueous supercapacitors and highlight the critical role of pore architecture—rather than extensive graphitic ordering—in maximizing capacitance in neutral buffered electrolytes.

Keywords

Activated carbon, Biomass-derived carbon, Birch wood, NaOH activation, Pore structure, Supercapacitors, Aqueous electrolyte

Acknowledgements

This project, titled Atomic Layer-coated Graphene Electrode-based Micro-flexible and Structural Supercapacitors (grant agreement ID 101120677), is supported by the European Commission's Horizon Europe programme and forms part of the Graphene Flagship initiative, which aims to advance technologies using graphene and other two-dimensional materials.

Ferroelectrics and Functional Materials

Molten salt synthesis towards preparation of Ruddlesden-Popper, perovskite and pyrochlore-type materials

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The synthesis of complex oxide materials such as Ruddlesden-Popper, perovskite, and pyrochlore structures is commonly performed using the conventional solid-state reaction method. Although this technique is widely used due to its simplicity and scalability, it typically requires high reaction temperatures, long calcination times, and repeated grinding steps to achieve phase purity and homogeneity. These limitations often lead to poor control over particle size, morphology, and final product composition. As an alternative, molten salt synthesis has emerged as an efficient route for the preparation of complex inorganic materials. In this method, a molten salt medium acts as a high-temperature solvent that enhances ion diffusion and mass transport, thereby significantly accelerating solid-state reactions. As a result, the formation of crystalline phases can occur at lower temperatures and shorter reaction times compared with conventional solid-state synthesis. Additionally, molten salt synthesis can provide improved control over particle morphology and crystallinity.

Many synthesis parameters, including reaction time, temperature, the nature of the materials used, ratio between salts and starting materials, can be adjusted, which could lead to selective formation of various phases. In one of our works [1], we synthesized three different Y-Mn-O structures, like $Y_2Mn_2O_7$ pyrochlore, orthorhombic or hexagonal $YMnO_3$ by adjusting the reaction temperature and ratio between Y and Mn nitrates to NaCl-KCl mixture. Another study [2] revealed that four different Ruddlesden-Popper phases can be prepared by adjusting the reaction temperature, as well as the ratio of starting materials to chloride salts.

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Keywords

Molten salt synthesis, perovskites, pyrochlores, Ruddlesden-Popper

Materials for Photonics

Broadband near-infrared Cr3+ luminescence in Zn2+/Zr4+-modified Gd3Ga5O12 garnet

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Near-infrared (NIR) radiation has applications in medicine, anti-counterfeiting, night vision, and non-destructive food analysis. Recently, near-infrared phosphor-converted light-emitting diodes (NIR pc-LEDs) with broadband emission have shown potential as NIR sources; however, they still exhibit significant drawbacks, including relatively low quantum efficiency and poor thermal stability. In this work, we investigate the optical properties of gadolinium gallium garnet (GGG) phosphors, $Gd_3Ga_5O_{12}:Cr^{3+}$, with a modified structure achieved by incorporating Zn^{2+}/Zr^{4+} ions.

Polycrystalline materials with the composition $Gd_3Ga_{5-2x}Zn_xZr_xO_{12}:0.05Cr$ (x = 0–1) were synthesized from high-purity raw materials using the solid-state reaction method at 1300 °C for 6 h in air. Phase purity of the samples was examined by X-ray diffraction. Optical properties were investigated using diffuse reflectance, photoluminescence excitation and emission, and decay kinetics measurements.

Powder X-ray diffraction confirmed the incorporation of Zn and Zr into the GGG structure. Diffuse reflectance and excitation spectra revealed a red shift of Cr^{3+} absorption and excitation bands with increasing Zn/Zr content. Increasing Zn/Zr concentration caused the broad Cr^{3+} luminescence band to shift from 730 nm to 805 nm under 450 nm excitation. At the same time, the full width at half maximum (FWHM) increased from 100 to 180 nm, resulting in improved coverage of the NIR spectral range important for NIR applications.

Keywords

Near-infrared luminescence; Cr3+ phosphors; Garnet phosphors; Phosphor-converted LEDs; Broadband emission

Acknowledgements

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Ferroelectrics and Functional Materials

Electromechanically responsive materials based on electrospun polymer nanofibers

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Polyvinylidene fluoride (PVDF) is a crucial piezoelectric electromechanically responsive polymer for a wide range of applications, such as flexible tactile, force and deformation sensors or mechanical energy harvesters. However, the synthesis of PVDF requires the use of per- and polyfluorinated alkyl substances (PFAS) known colloquially as 'forever chemicals'. As such, there is a pressing need to develop alternative environmentally friendly flexible polymer transducer technologies [1]. Recently, the electromechanically responsive electrospun laminate approach was demonstrated [2], involving various types of polymers, thus providing ample room for further improvements or functionalities such as stretchability, biodegradability, or biocompatibility.

Usually, "direct" effect is investigated and reported in literature for such flexible polymer systems - the generation of electrical charge (voltage) when mechanical stress, pressure, or vibration is applied to them. Here we demonstrate the converse phenomenon – mechanical deformation in response to an applied electric field. Samples with a large density of interfaces per volume have been made by electrospinning nanofibres from different polymers. Standard AixACCT TF2000 analyzer setup allowed us to measure the polarization of the samples as well as mechanical deformation due to the applied electric field and to identify the nature of electromechanical response (i.e. electrostrictive or piezoelectric). In several systems we were also able to induce piezoelectric like response using special electrode configurations and applied high voltages.

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Keywords

piezoelectric, polymer, transducer, nanofibres

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Materials for Photonics

Laser processing as an alternative route for obtaining electroluminescent ZnS:Cu

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Alternating-current powder electroluminescent (ACPEL) thick-films based on ZnS phosphors are promising for large-area and flexible light-emitting devices. Their performance strongly depends on phosphor activation and processing conditions, while conventional thermal treatment may limit compatibility with polymer composites.

In this work, laser-assisted powder processing is explored as a preliminary route for preparing ZnS:Cu-containing luminescent material. ZnS powder was combined with a copper precursor and subjected to laser treatment. The obtained material was evaluated by photoluminescence spectroscopy and compared with a reference ZnS:Cu phosphor prepared by microwave-assisted synthesis followed by thermal activation.

The laser-treated powder showed visible green emission under UV excitation and a broad photoluminescence band comparable to the reference material. To evaluate electroluminescence possibility, the powder was incorporated into a polyurethane composite film and used to fabricate a preliminary ACPEL panel. Weak electroluminescence was detected under AC excitation, demonstrating proof-of-concept device operation.

These results indicate that laser-assisted powder processing can produce optically active ZnS:Cu-containing material for preliminary ACPEL device fabrication. Further optimization of laser parameters, material yield, dopant activation, and composite film preparation is required to improve electroluminescent performance.

Keywords

Zinc Sulphide, laser processing, AC Electroluminescence, ACPEL

Acknowledgements

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Materials for Energy, Materials for Photonics, Theoretical Modeling of Functional Materials and Devices

Simulation of conductive networks in nanotube-based composites

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Nanocomposites exhibit enhanced mechanical and electrical properties by incorporating nanotubes, such as carbon nanotubes, into an insulating matrix. In our simulations, we introduce a tunneling range: when the shortest distance between two nanotubes falls within this range, a tunneling contact forms, enabling electrical conductivity [1].

The system is modeled as a graph, with percolation determined by identifying the connected component that spans opposite faces of the simulation box, which serve as “electrodes” represented by zero-dimensional pseudo-tubes. Conducting clusters are found using a weighted quick-union algorithm with path compression. For each configuration, approximately 20 simulations were run under identical parameters, and the percolation threshold was calculated as their average.

This approach produces a robust three-dimensional model [2] that accurately describes the formation of conductive nanotube networks, accounting for the tunneling mechanism of electrical conduction. Results show that increasing the system size or the number of simulations improves percolation threshold accuracy and agreement with experimental data. A “soft-core” model without tunneling does not yield reliable results. Furthermore, increasing the nanotube alignment angle generally lowers the percolation threshold, with the most significant effect observed at 30–50°.

These findings provide a quantitative framework for predicting percolation in nanotube-based composites and highlight the critical roles of tunneling contacts and nanotube orientation in forming conductive pathways.

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Keywords

Nanocomposites, carbon nanotubes, percolation threshold, electrical conductivity, tunneling effect

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Materials for Energy, Materials for Photonics, Theoretical Modeling of Functional Materials and Devices

Characterization of Free Volume Transformations in MgAl2O4 Ceramics

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This study applies positron annihilation lifetime spectroscopy to investigate free nanovolumes in humidity-sensitive MgAl2O4 ceramics using multicomponent positron–positronium trapping models [1]. The results indicate that these ceramics exhibit two components in PALS measurements: the first component (τ1, I1) reflects the material's microstructural properties, while the second component (τ2, I2) is associated with volume defects near intergranular boundaries, formed by secondary phases within the ceramic structure. Another measurement channel reveals a single component (τ3, I3), corresponding to ortho-positronium (o-Ps) annihilation via the “pick-off” process in nanopores.

Further PALS investigations on modified MgAl2O4 ceramics under dry and wet conditions with high-statistical accuracy allowed detailed analysis of these components. In the second channel, two components (τ3, I3) and (τ4, I4) describe o-Ps decay within nanopores. The first component (τ3, I3) corresponds to o-Ps annihilation in nanopores approximately 0.2–0.3 nm in size, with increased intensity in the presence of water. The second component (τ4, I4) represents o-Ps annihilation in larger pore volumes (≈1.8–2 nm radius), where water molecules form a layer on the pore walls.

Thus, the multicomponent positron–positronium model effectively describes the transformation of free volumes in materials with well-developed porous structures, providing deeper insight into the influence of humidity on ceramic nanopores.

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Keywords

MgAl2O4 ceramics, nanopores, free volumes, humidity effects, multicomponent model

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Materials for Energy, Materials for Photonics, Ferroelectrics and Functional Materials

Grains and crystallite size study of the optically transparent spinel ceramics

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To ensure transparency, the ceramic must be sintered from a homogeneous, single-phase material with negligible optical absorption, whose crystalline structure provides isotropic optical properties. It must also be dense and consist of grains significantly smaller than the wavelength of light and contain no pores that cause refraction or scattering of light. The magnesium-aluminium spinel $MgAl_2O_4$ (MAS) has a cubic crystal structure and is characterised by a very wide bandgap, which provides its transparency across the spectrum from UV to IR. Thus, the transparency of MAS polycrystalline ceramics depends primarily on its microstructure, which, in turn, is determined by the sintering process.

This study focuses on the investigation of MAS-type ceramics sintered using the high-pressure-high-temperature (HPHT) method from micro-powders obtained by solid-phase synthesis from MgO and Al_2O_3 powders at a temperature of 1500 °C in air. The microstructure of the powders and ceramics was investigated using scanning electron microscopy, and the size of the crystallites was estimated from the broadening of the X-ray diffraction peaks.

Although the particle size of the micro-powder after synthesis was well over 1 μm, after sintering the ceramic became transparent and the grain size was reduced to about 80-100 nm. On the other hand, the size of the crystallites that make up the ceramic grains was even smaller.

Keywords

MgAl2O4, spinel, optical transparency, ceramics, microstructure

Acknowledgements

The study has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (GA No 101052200 EUROfusion) and was partially co funded by the Polish Ministry of Science and Higher Education (project No 602430) and the Ukrainian-Latvian Joint Programme of Scientific and Technological Cooperation (projects 0125U003462 and LV-UA/2025/12).

Materials for Photonics, Ferroelectrics and Functional Materials, Technologies and Devices

Effect of Eu^{3+} doping on free-volume defect structure of $BaGa_2O_4$ ceramics

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$BaGa_2O_4$ ceramics are considered promising materials for optoelectronic applications, particularly as insulating layers and secondary coatings in plasma display panels. Doping with rare-earth ions can significantly modify the structural and functional properties of these ceramics. The aim of this work is to study the evolution of internal free volumes, including extended defects and nanopores, in $BaGa_2O_4$ ceramics doped with Eu^{3+} ions using positron annihilation lifetime (PAL) spectroscopy. $BaGa_2O_4$ ceramics were synthesized by a solid-state reaction from $BaCO_3$ and Ga_2O_3 with Eu_2O_3 additions of 1, 3, and 4 mol% [1]. PAL measurements were performed using an ORTEC spectrometer with a ^{22}Na positron source at 22 °C and relative humidity of 35%. The obtained spectra were analyzed with the LT program using a four-component fitting procedure typical for porous ceramic structures. Two main annihilation channels were observed: positron trapping at bulk defects and annihilation via ortho-positronium decay. The shortest lifetime component reflects the microstructure of the main phase, while the intermediate component is related to free-volume defects near grain boundaries. The longer components correspond to nanopores and their evolution. Additional phases located mainly at grain boundaries create defect centers acting as positron traps. The results show that increasing Eu^{3+} concentration from 1 to 3 mol% causes agglomeration of free-volume defects near grain boundaries and an increase in nanopore size and concentration. Further increase of Eu^{3+} content leads to fragmentation of free-volume defects and nanopores in the ceramic structure.

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Keywords

$BaGa_2O_4$ ceramics, Eu^{3+} doping, free-volume defects, nanopores

Acknowledgements

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Microfluidics and Biomedical technologies

Studying magnetotactic bacteria dynamics in porous media by using microfluidic chips

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Understanding bacterial dynamics in porous environments is crucial in agriculture and medicine, where predicting bacterial spread supports plant growth promotion [1] and cancer-related applications [2]. While passive transport is well captured by established porous-media models [4], a key gap remains in predicting how active bacteria move through complex matrices. Magnetotactic bacteria (MTB), such as *Magnetospirillum gryphiswaldense*, naturally synthesize magnetic nanoparticles (magnetosomes) that enable navigation along geomagnetic fields lines. This makes them an attractive model system: they are intrinsically active and, at the same time, unique amenable to external guidance for controlled navigation [3]. In this study we investigated the navigational capabilities of *M. gryphiswaldense* as they traverse obstacle arrays under controlled magnetic fields. We will use PDMS microchannels engineered with a dense micropillar array, creating a well-defined obstacle-rich microstructure [3] Bacterial transport through the chip is visualized via microscopy using a high-speed camera under different applied magnetic field. The transport efficiency to the collection point for both strains across magnetic field strengths is being quantified, comparing mutant and wild-type performance to disentangle the contributions of motility versus magnetotactic guidance. Learning these parameters will provide important understanding of optimal control conditions for further development of bio-microbots.

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Keywords

Magnetotactic bacteria, Magnetospirillum gryphiswaldense, microfluidics, porous media, flagellar mutant.

Acknowledgements

Micro and Nanodevices Laboratory - ISSP-UL

Theoretical Modeling of Functional Materials and Devices

Advanced modeling methods to investigate oxygen defects in MgO

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Radiation-induced Frenkel defects greatly affect the basic properties of wide bandgap materials such as MgO (=7.8 eV). However, some questions regarding the thermal stability of oxygen defects in MgO still remain open and require further investigation [1]. In particular, the mobility of oxygen interstitials () governs the thermal annealing of Frenkel defects and needs a deeper atomistic understanding. In this context, the density functional theory (DFT) calculations represent a powerful tool to analyze the behavior and implications of such defects. In the present study, the meta-GGA functional is employed to investigate the oxygen defects in MgO, in order to advance their understanding. Our approach is to separately treat oxygen vacancies in different charge states (i.e., *F*- and F^+-centers) and interstitials in different charge states, to analyze experimental defect annealing kinetics. Supercell size effects (up to 216 atoms) are systematically examined to properly account for electrostatic defect interactions in charged supercells. First, we combine and compare two types of basis sets for the calculations of *F*-type centers in MgO, namely Gaussian-type and plane wave basis sets, with the functionals. Secondly, we apply machine learning force field and nudged elastic band methods within the plane wave framework to determine the details and mechanisms of migration and their dynamical behavior. Finally, we present the analysis of oxygen defect formation energies and electronic properties.

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Keywords

MgO, radiation defects, oxygen vacancies and interstitials, DFT, meta-GGA, MLFF

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Materials for Energy

A comparative study of YAP:Bi and YAP:Mn phosphors: X-ray-, photo-luminescence and OSL response to irradiation

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Phosphors based on yttrium-aluminium perovskite $YAlO_3$ (YAP) have a relatively high effective atomic number Z_{eff}. This, in particular, allows YAP:Mn to be used in passive luminescent dosimetry via thermoluminescence (TLD) and optically stimulated luminescence (OSL) methods, in combination with a tissue-equivalent phosphor for the detection of unknown radiation [1], as well as for the X-ray imaging technology for medical diagnostics. However, YAP:Mn single crystals, whilst being an excellent phosphor for TLD [2], have certain drawbacks in OSL dosimetry due to prolonged afterglow following irradiation [3].

This study is devoted to a comparative investigation of the new YAP:Bi phosphor and YAP:Mn phosphor with regard to their potential use as storage dosimetric materials for OSL dosimetry. In particular, its photoluminescence, X-ray luminescence, phosphorescence and OSL peculiarities are compared. It has been shown that, given its overall luminescent properties, YAP:Bi offers significant advantages as a phosphor for optically stimulated luminescence (OSL) dosimetry.

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Keywords

YAlO3, storage phosphor, luminescence dosimetry, optically stimulated luminescence

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Materials for Energy

Influence of Chamber Wall Thickness on the Thermal Performance of a Liquid Piston Hydrogen Compressor

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Hydrogen compression is an essential process in hydrogen storage and refuelling systems [1]. Liquid piston compressors are considered a promising alternative to conventional mechanical compressors due to reduced leakage and friction losses, as well as favourable heat-transfer conditions. Our previous studies addressed thermodynamic processes in the compression chamber and the influence of chamber dimensions on the behaviour of a liquid piston hydrogen compressor [2,3].

In the present work, the influence of chamber wall thickness on transient heat transfer during hydrogen compression was investigated numerically. A two-dimensional axisymmetric multiphysics model was used to simulate a single compression stroke in a liquid piston hydrogen compressor. The analysis was performed for initial hydrogen pressures of 3–20 MPa, stroke durations of 0.5–20 s, and chamber wall thicknesses of 2.5, 5.0, and 10.0 mm.

The results show that the chamber wall temperature rise increases with increasing initial pressure and compression time, while increasing wall thickness reduces the per-stroke temperature increase due to higher thermal inertia. The temperature distribution in the chamber wall is non-uniform, and the highest thermal loading is observed in the upper part of the chamber exposed to compressed hydrogen. Under the investigated conditions, the wall temperature rise reached about 9.6 K for a 2.5 mm wall and about 2.2 K for a 10.0 mm wall at 20 MPa and a 20 s compression stroke.

The obtained results show that chamber wall thickness is an important design parameter affecting thermal behaviour and heat dissipation in liquid piston hydrogen compressors. These findings are useful for further optimization of hydrogen compression systems for high-pressure applications [4].

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Keywords

hydrogen compression; liquid piston compressor; CFD modeling; numerical simulation; heat transfer

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Materials for Photonics

Excitonic and defect-related luminescence in $BaMgF_4$ ceramics under VUV excitation

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The luminescence properties of $BaMgF_4$ ceramics synthesized via electron beam-assisted synthesis were investigated under vacuum ultraviolet (VUV) synchrotron excitation. The study was performed in the excitation energy range of 4–10.8 eV at a cryogenic temperature of 9 K in order to suppress non-radiative relaxation processes and reveal intrinsic luminescence mechanisms.

The synthesized ceramics exhibited high phase purity (~99.3%) with an orthorhombic crystal structure and an average crystallite size of ~41 nm. Energy-dispersive spectroscopy confirmed the presence of Ba, Mg, and F, with slight fluorine deficiency indicating the formation of defect centers [1].

Photoluminescence spectra showed a broad emission band in the 300–550 nm range with distinct maxima at 336, 372, 420, and 470 nm. The dominant emission peak at 336 nm was attributed to self-trapped excitons (STE) formed near the band edge under high-energy excitation (~9.3–9.7 eV). Additional emission bands at ~3.0 eV and ~2.8 eV were associated with defect-related states efficiently excited at intermediate energies (6.45 and 8 eV).

The excitation spectra revealed pronounced maxima at 5, 6.45, and 8 eV, corresponding to defect-related electronic transitions, as well as high-energy interband excitation processes near 10.3 eV. The results demonstrate a complex interplay between excitonic recombination and defect-induced luminescence mechanisms.

The study confirms that radiation-assisted synthesis introduces intrinsic defects that significantly influence the luminescent behavior of $BaMgF_4$ ceramics. These findings highlight the potential of this material for applications in UV/VUV photonics, scintillation detectors, and nonlinear optical devices.

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Keywords

$BaMgF_4$, luminescence, VUV excitation, excitons, defects

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Materials for Photonics

Structural Disorder and Radiation Damage in $ZnGa_2O_4$ Spinel Ceramics under 231 MeV Xe Ion Irradiation

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Zinc gallium oxide spinel $ZnGa_2O_4$ is a promising radiation-resistant wide-band-gap oxide for optoelectronic, scintillation, and phosphor applications due to its stable cubic spinel structure and defect-sensitive luminescence.

In this work, $ZnGa_2O_4$ ceramics synthesized by the solid-state reaction method were studied before and after irradiation with 231 MeV Xe ions at fluences from 10^{11} to 10^{13} ions/cm^2. X-ray diffraction confirmed that the pristine ceramic is mainly represented by the cubic spinel $ZnGa_2O_4$ phase with space group Fd3m. The initial lattice parameter was a = 8.3352 Å, while after irradiation its gradual increase indicated radiation-induced lattice expansion and defect accumulation. No clearly resolved secondary crystalline phase was detected, showing that the spinel framework is generally preserved. However, diffraction peak broadening and a decrease in coherent scattering domain size indicate progressive structural disordering. Williamson–Hall analysis showed that the apparent crystallite size decreases from about 42 nm in the pristine sample to very low values at high fluence, while microstrain increases up to about 9.4% at 10^{13} ions/cm^2. This reflects severe peak broadening caused by high defect density, internal strain, and partial amorphization.

SRIM calculations showed that electronic stopping dominates over nuclear stopping, with values of about 32.45 and 0.106 keV/nm, respectively. The projected ion range is approximately 11.7 μm. The combined XRD and SRIM results indicate that high-energy Xe irradiation produces dense ionization tracks, promotes defect accumulation, increases lattice strain, and gradually disorders the $ZnGa_2O_4$ structure while preserving the spinel phase.

Keywords

$ZnGa_2O_4$, XRD, defects

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Materials for Photonics

VUV Luminescence Study of $MgGa_2O_4$-Based Spinel Ceramics

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Magnesium gallium spinel $MgGa_2O_4$ is a promising wide-band-gap oxide for photonic and optoelectronic applications due to its chemical stability, radiation resistance, and defect-sensitive luminescence. $MgGa_2O_4$-based ceramics are also considered as self-activated phosphors and host matrices for rare-earth ions, since their emission is strongly affected by intrinsic defects, antisite disorder, and energy-transfer processes. VUV spectroscopy is especially useful for studying these materials because it probes fundamental electronic states, defect-related excitation channels, and radiative recombination mechanisms.

In this work, VUV luminescence of $MgGa_2O_4$ ceramics synthesized by the conventional solid-state reaction method was studied in the temperature range from 10 to 300 K. The emission spectra show broad blue luminescence bands centered near 2.9–3.0 eV, characteristic of self-activated recombination involving intrinsic lattice defects. According to the defect model, this emission is related to donor–acceptor pair recombination associated with oxygen vacancies and antisite defects, including MgGa and GaMg centers. The broad shape of the bands indicates strong electron–phonon interaction and structural disorder typical of spinel compounds. At low temperature, suppression of non-radiative relaxation channels results in higher luminescence intensity and narrowing of the emission band.

The results show that luminescence in $MgGa_2O_4$ ceramics is governed by intrinsic defects, antisite disorder, and impurity-related recombination channels. VUV excitation spectroscopy confirms the role of matrix-mediated energy transfer and reveals multiple excitation pathways responsible for efficient visible emission. These findings demonstrate the potential of $MgGa_2O_4$ ceramics for phosphor, dosimetric, and radiation-resistant photonic applications.

Keywords

$MgGa_2O_4$, luminescence, VUV excitation, excitons, defects

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Materials for Energy

The role of radiation-induced defect centres on spectroscopic properties of lithium orthosilicate, lithium metatitanate and their composites

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Nuclear fusion reactors require *in-situ* tritium breeding using lithium-containing materials to achieve fuel self-sufficiency. Lithium orthosilicate (Li_4SiO_4) and lithium metatitanate (Li_2TiO_3) have been extensively tested for tritium breeding in the Helium Cooled Pebble Bed (HCPB) blanket concept for nuclear fusion reactors [1].

In this study, the radiation-induced defect centres in Li_4SiO_4, Li_2TiO_3 and their composites were analysed. The samples were irradiated with X-rays, and the formed centres were characterised using electron paramagnetic resonance (EPR), X-ray-induced luminescence (XRL), photoluminescence (PL), and thermally stimulated luminescence (TSL) spectroscopy. The EPR analysis indicates that the paramagnetic centres are primarily formed in the Li_4SiO_4 phase and are related to multiple electron and hole-type centres. During X-ray excitation, broad host-related luminescence bands in the 300-600 nm range were observed in all samples. In Ti^{4+} containing hosts, additional luminescence bands in the red and near-infrared (650-800 nm) spectral range related to Mn^{4+} were detected and likely introduced from precursors and stabilised by Ti^{4+} ions. The obtained TSL glow curves for the irradiated samples indicate that the formed centres are annealed at temperatures up to 300 °C, with dominant glow peaks at 70 and 160 °C, which is consistent with the annealing behaviour observed for the EPR signals. The results indicate that the dominant defect-related spectroscopic responses are related to the paramagnetic centres formed in the Li_4SiO_4 phase.

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Keywords

Tritium breeding; Radiation-induced defect centres; Electron paramagnetic resonance, Thermally stimulated luminescence, X-ray-induced luminescence

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Materials for Photonics

Comparison of Microwave-Assisted and Laser-Activated Solid-State Sintering for Eu,Dy,B-Doped Strontium Aluminate Phosphors

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Eu,Dy-activated strontium aluminate is one of the most efficient long-persistent phosphors known today. It can absorb visible light and emit luminescence for several hours after excitation, which makes it suitable for applications such as safety signage, emergency lighting, and road markings. Conventionally, this material is synthesized using combustion methods, which require the use of fuels and lead to the release of gaseous by-products. Therefore, alternative synthesis approaches are of interest.

Various methods have been reported for the preparation of Eu,Dy,B-doped strontium aluminate, including solid-state synthesis, sol-gel processing, and microwave-assisted synthesis. However, direct comparisons of different sintering techniques are still limited in the literature. In this work, two synthesis approaches are compared: microwave-assisted synthesis followed by sintering in a reducing atmosphere, and laser-activated solid-state sintering.

The crystalline phases of the obtained materials were identified using X-ray diffraction (XRD), while the morphology of the samples was examined by scanning electron microscopy (SEM). Photoluminescence emission spectra and decay kinetics were measured to evaluate the optical properties of the phosphors. Luminescence in the 500–520 nm range was observed, corresponding to the Eu^{2+} transition ($4f^6 5d^1 \rightarrow 4f^7$). The structural, morphological, and luminescence properties of the samples were analyzed to compare the effectiveness of the two synthesis methods.

Keywords

long-lasting luminescence, microwave synthesis, laser sintering

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Materials for Photonics, Ferroelectrics and Functional Materials

LUMINESCENCE OF Tb/Eu3+-DOPED Y2.97-xNaxAl5O12 GARNETS UNDER SYNCHROTRON RADIATION

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Garnets are well-known phosphor host materials for various applications in modern optics and photonics. Recently, novel multicomponent garnets containing potassium or sodium and activated by RE^{3+} ions have been studied as potential phosphors [1,2]. It has been shown that luminescence properties of $Y_{2.97-x}K_x(Eu,Tb)_{0.03}Al_5O_{12-y}$ compounds worsen with increasing K content due to the formation of nonradiative recombination centers [2]. Here, we present the first results of the luminescence study in a wide energy range (2.5-45 eV) of Tb^{3+}/Eu^{3+}-doped YAG modified by Y substitution with Na.

A set of single-phase $Y_{2.97-x}Na_xTb_{0.03}Al_5O_{12}$ and $Y_{2.97-x}Na_xEu_{0.03}Al_5O_{12}$ (x = 0.03-0.6) compounds with garnet-type structure were synthesized for the first time using the sol-gel method. Luminescent spectroscopy in the UV-VUV region was performed using the laboratory setups and photoluminescence endstation of the FinEstBeAMS beamline at the MAX IV synchrotron facility. The luminescence spectra of the studied samples under VUV excitation are characterized by a typical set of peaks in the visible range, which correspond to intraconfigurational $^5D_0$-^7F_J (J = 1,2,3,4) and $^5D_3$,$^5D_4$-^7F_J (J = 6,5,4,3,2) transitions in Eu^{3+} and Tb^{3+} ions, respectively. It is shown that yttrium substitution by sodium results in the increase of emission intensity with Na^+ content. The efficiency of energy transfer from the host to the emission centers, as well as temperature effects, is analysed.

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Theoretical Modeling of Functional Materials and Devices

The effective diffusion coefficient in inhomogeneous solids with inclusions. A comparison of 2D continous and discrete models

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Transport in nanomaterials remains challenging problem. We considered the effective diffusion coefficient D_{eff} in solids with periodically distributed impenetrable square inclusions (holes) with fraction f using 2D continuous and discrete lattice models. For the continuous case, the results of modified Maxwell theory (effective medium approximation) [1] are compared with those in the form of an explicit formula for the effective thermo-conductivity [2] (homogenization theory). In both continuous models $D_{eff}(f)$ dependences on f coincide within 2-3 percent. However, continuous models do not explain the transition from two-dimensional diffusion to one-dimensional one, along the one - dimensional channels in the limit of large square holes. The boundary values $Deff(f=1)/D_2$=0.5 (where D_2 is the host diffusion coefficient) for continuous models are explained based on the discrete approach: two-dimensional lattice (lattice constant l) with periodically (period L) placed square holes. It is shown that contrary to the continuous diffusion approximation in 2D dependence of effective diffusion coefficient D_{eff} of f is not a monotonously decreasing function (see Figure). If hopping along the L square contours are permitted in limiting case, when f tends to 1, $Deff$ tends to host diffusion coefficient D_2. $D_{eff}(f)$ analytical dependence near f=1 can be received from simple considerations. $D_{eff}(f)$ dependence on f in a whole range [0,1] is obtained in computer simulations for the discrete case varying L values up to L=500l. Computer simulations confirm analytical theory.

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Keywords

Difusion coefficient, Discrete and continuous models, Computer simulation

Acknowledgements

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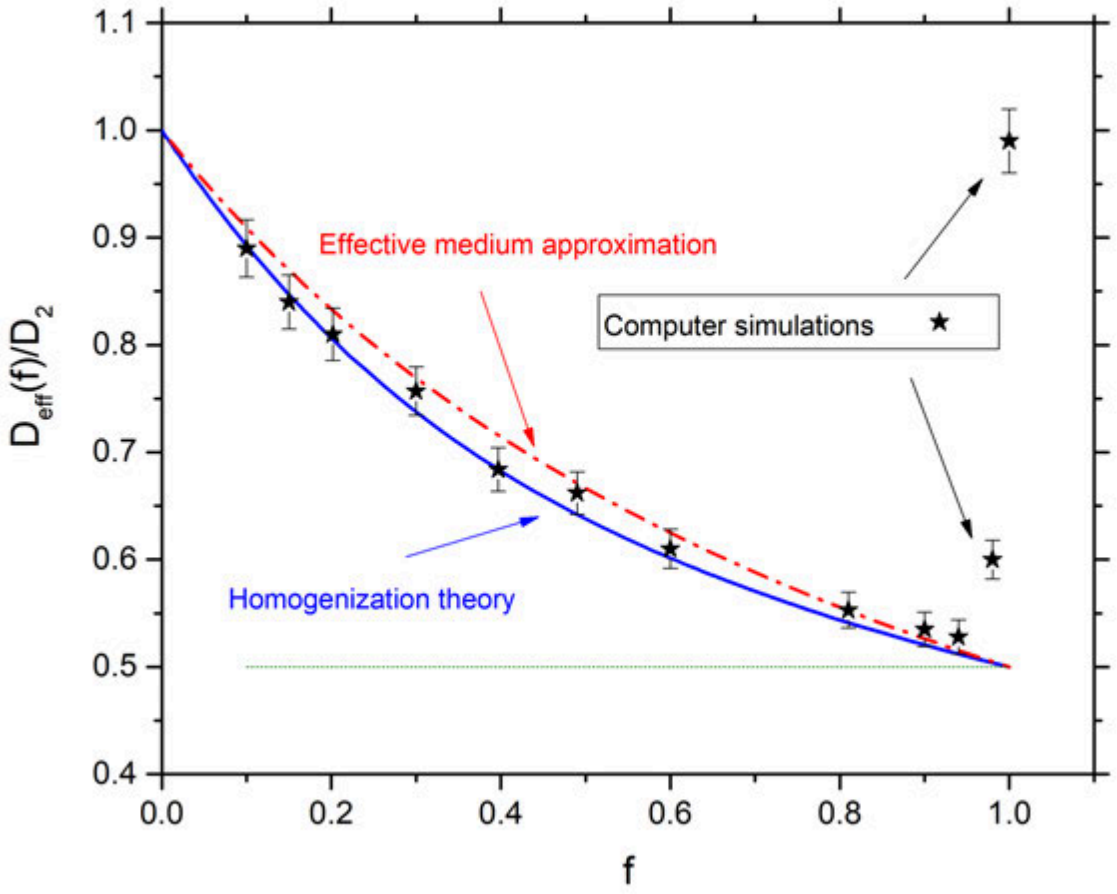
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$D_{eff}(f)/D_2$
Effective medium approximation
Computer simulations
Homogenization theory

Ferroelectrics and Functional Materials

Impact and characteristics of oxygen vacancies in ferroelectric HfO2 based materials

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The stabilization of the polar orthorhombic phase in hafnium oxide (HfO_2) is critically influ-enced by the presence and behavior of oxygen vacancies, which play a key role in the ferroe-lectric properties of the material. In this study, we investigate the nature, concentration, and charge states of oxygen vacancies in undoped and doped HfO_2 nanoparticles using a combi-nation of complementary structural and spectroscopic techniques. X-ray diffraction (XRD) is employed to identify phase composition and assess the structural stability of the orthorhom-bic phase, while thermostimulated luminescence (TL) provides insights into the activation energies and trap states associated with defect centers. X-ray photoelectron spectroscopy (XPS) is used to quantify vacancy charge states and analyze the local electronic environment of dopants and oxygen-deficient sites. Extended X-ray absorption fine structure (EXAFS) spectroscopy allowed determination of coordination numbers and local atomic arrangements around hafnium and dopant atoms. Through this multi-technique approach, we determined oxygen vacancy concentrations, coordination numbers, and activation energies for both pure and doped HfO_2 systems. The results reveal how specific dopants influence vacancy for-mation and stabilization mechanisms, providing a deeper understanding of how defect chem-istry governs the persistence of the polar orthorhombic phase in hafnia-based ferroelectric materials.

Keywords

HfO2, ferroelectric, defects, oxygen vacancies

Acknowledgements

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Materials for Photonics

Fabrication of strongly coupled cavity arrays using grayscale UV lithography

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Strong light–matter coupling underpins emerging technologies in polaritonics, enabling hybrid states that combine photonic and excitonic properties, that are central to emerging technologies such as low-threshold polariton lasers, quantum simulators, and ultrafast optical switches – yet scalable fabrication methods remain limited. [1], [2], [3], [4], [5]

In this study, we demonstrate the fabrication of large-scale arrays of dye-doped, strongly coupled Fabry–Pérot (FP) cavities using grayscale UV lithography. By blending the photoresist AR-P3510T with varying concentrations of Rhodamine 6G dye, we systematically investigated the impact of dye concentration on lithographic performance, including defect formation and cavity uniformity. To our knowledge, this represents the first successful use of grayscale UV lithography for the scalable production of strongly coupled FP cavity arrays, offering significant advantages over conventional fabrication techniques in terms of throughput and tunability. [6], [7]

Our approach enabled the creation of hundreds to thousands of strongly coupled FP cavities, with the potential to accelerate fundamental research in strong light–matter coupling. Beyond basic studies, this method also provides a promising route for on-chip fabrication of polaritonic cavities, paving the way toward compact laser-like light sources and novel integrated polaritonic devices.

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Keywords

Fabry-Pérot resonators, polaritons, grayscale lithography, R6G dye-doping

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Materials for Energy

Discovery of photochromism with fast bleaching in oxygen-containing lanthanum hydride thin films

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Emija Letko , Institute of Solid State Physics, University of Latvia
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Anatolijs Sarakovskis , Institute of Solid State Physics, University of Latvia
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Oxygen-containing rare-earth hydrides (REHOs), including those based on yttrium, gadolinium, dysprosium, and erbium, exhibit a heliochromic photochromic effect, making them promising materials for smart window applications [1]. Although REHO thin films have been actively studied over the past decade, some rare-earth elements, including lanthanum (La), have not yet been investigated for their photochromic properties. This study reports, for the first time, the fabrication of photochromic LaHO thin films by reactive magnetron sputtering in an argon–hydrogen atmosphere, followed by controlled oxidation and encapsulation with aluminium nitride and aluminium oxide layers to improve stability.

The thin films were characterized using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and a custom-built system for photochromic measurements. In particular, the influence of post-deposition oxidation time on optical properties and crystal structure was investigated.

Structural analysis revealed a textured, polycrystalline cubic LaHO phase with lattice parameters of 5.65–5.76 Å and significant oxygen incorporation, with an O/La atomic ratio of ~1, confirmed by both XRD and XPS.

The films exhibited average transmittance up to 78% in the 500-700 nm range. Under 10 minutes of solar-simulated illumination, LaHO films showed reversible photodarkening in the same spectral region, with relative optical contrast tunable between ~6% and 17%. Fast bleaching was also observed, with effective time constants of 0.6-1.4 minutes.

These results confirm the photochromic nature of LaHO thin films, with properties comparable to other REHOs, identifying LaHO as a new member of the oxygen-containing rare-earth hydride family.

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Keywords

Smart windows, Photochromism, Oxygen-containing rare-earth hydrides

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Materials for Photonics, Theoretical Modeling of Functional Materials and Devices

Coupling between MoS2 and Plasmonic grating

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Chiao-Chih LIN , National Cheng Kung University
Wing-Sing Cheung , National Cheng Kung University
Po-Han Wang , National Cheng Kung University

This work demonstrates a semiconductor–insulator–metal (SIM) light-emitting device integrating monolayer transition metal dichalcogenides and nano plasmonic structures. High-quality 2D materials were prepared by mechanical exfoliation and dry transfer[1]. Plasmonic nanostructures, designed via finite element method (FEM) to match emission wavelengths. Angle-resolved Reflectance shows the dispersion of the grating. To characterize the optical properties of the device, angle-resolved spectroscopy was employed. The reflected and emitted light from the sample was collected through home-built Fourier optical measurement system[2], and the dispersion behavior was obtained as a function of incident or detection angle.

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Keywords

2D materials, Surface plasmon resonance, Nanoscale light-emitting device, Simulation

Acknowledgements

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Technologies and Devices

Close-loop wavefront pre-compensated laser amplifier for structured light amplification

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Saulius Tumenas , Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania
Sergej Orlov , Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania
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Evelina Dudutiene , Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania
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As laser technology advances, precise control of frequency, polarization, and spatiotemporal phase has greatly expanded the use of structured light in scientific and industrial applications. In laser micromachining, vortex beams reduce ablation thresholds for pillar fabrication on tantalum[1], while Bessel-like beams enable high-precision processing of transparent materials due to their extended depth of focus[2]. However, high power structured beam generation remains challenging because ablation level fluence (0.1 - 10 J/cm^2) is incompatible with LC-SLM handling limits, and mode amplification is sensitive to nonlinear effects and system aberrations. To overcome these constraints, we demonstrate a close-loop wavefront-precompensated structured light laser amplifier that enables power scaling with robust mode preservation and dynamic mode switching.

A LC on silicon-SLM shapes a 1030 nm Gaussian seed into structured modes using a weighted Gerchberg Saxton algorithm[3]. These modes are amplified in a 10 pass Yb:YAG thin disk amplifier pumped at 969 nm to reduce thermal loading[4]. A sampled output is imaged onto a CCD to monitor beam fidelity, and deviations from the target profile are fed back to compute corrective phase pre-compensation. Closed loop wavefront control is implemented using an SPGD algorithm with a Zernike basis to mitigate power dependent distortions[5]. This approach restores undistorted Gaussian and vortex modes with over 92% intensity correlation across 50 to 300 W pump power, while improving Gaussian beam gain by ~20% due to enhanced mode overlap. These results demonstrate scalable, adaptive structured beam amplification, with extension to high energy pulsed operation (>100 \mu J) currently underway.

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Keywords

structured light, laser amplifier, wavefront pre-compensation

Acknowledgements

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Materials for Energy, Large-Scale Research Infrastructures, Science Policy and Collaboration

Short-range structural distortions in (MgCoNiCuZn)O high-entropy oxide revealed by EXAFS spectroscopy

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High-entropy oxides represent a broad class of compounds in which five or more elements share a common cation sublattice with equal or near-equal probability (see figure) [1]. The constituent elements can be selected deliberately, tuning or fundamentally altering the properties of the compound. In this study, we investigate the high-entropy oxide (MgCoNiCuZn)O, first reported by Rost et. al. [2].

Polycrystalline (MgCoNiCuZn)O was synthesized by co-precipitation from equimolar aqueous solution of Mg, Co, Ni, Cu and Zn acetates, and NaOH aqueous solution. The resulting precipitate was filtered, washed with de-ionized water, and dried overnight in room temperature. The dry powder was then heated at 950°C for 8 hours.

X-ray diffraction combined with Rietveld analysis confirms a single-phase cubic rock-salt Fm-3m (226) structure with a lattice parameter of a = 4.2400(2) Å. In the Raman spectrum, one-phonon scattering, observed as a broad band at 550 cm^{-1}, suggests strong local disorder [3], similar to that observed in NiO-MgO solid solutions [4].

Temperature-dependent (10-300 K) X-ray absorption experiments were performed at the Co, Ni, Cu, and Zn K-edges in transmission mode at the DESY PETRA III P65 beamline [5]. The local atomic structure around the absorbing atoms was determined using multi-edge reverse Monte Carlo simulations [6]. The metal atoms in (MgCoNiCuZn)O exhibit octahedral coordination by six oxygen atoms. While NiO_6 and ZnO_6 octahedra show only weak distortion, Cu exhibits clear evidence of first-order Jahn-Teller distortion, consistent with the Cu^{2+} oxidation state and previous report [2]. A local distortion around the Co atoms is also observed; it was proposed previously in [2] but has not been demonstrated experimentally until now.

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Keywords

High-entropy oxides, (MgCoNiCuZn)O, EXAFS, reverse Monte Carlo

Acknowledgements

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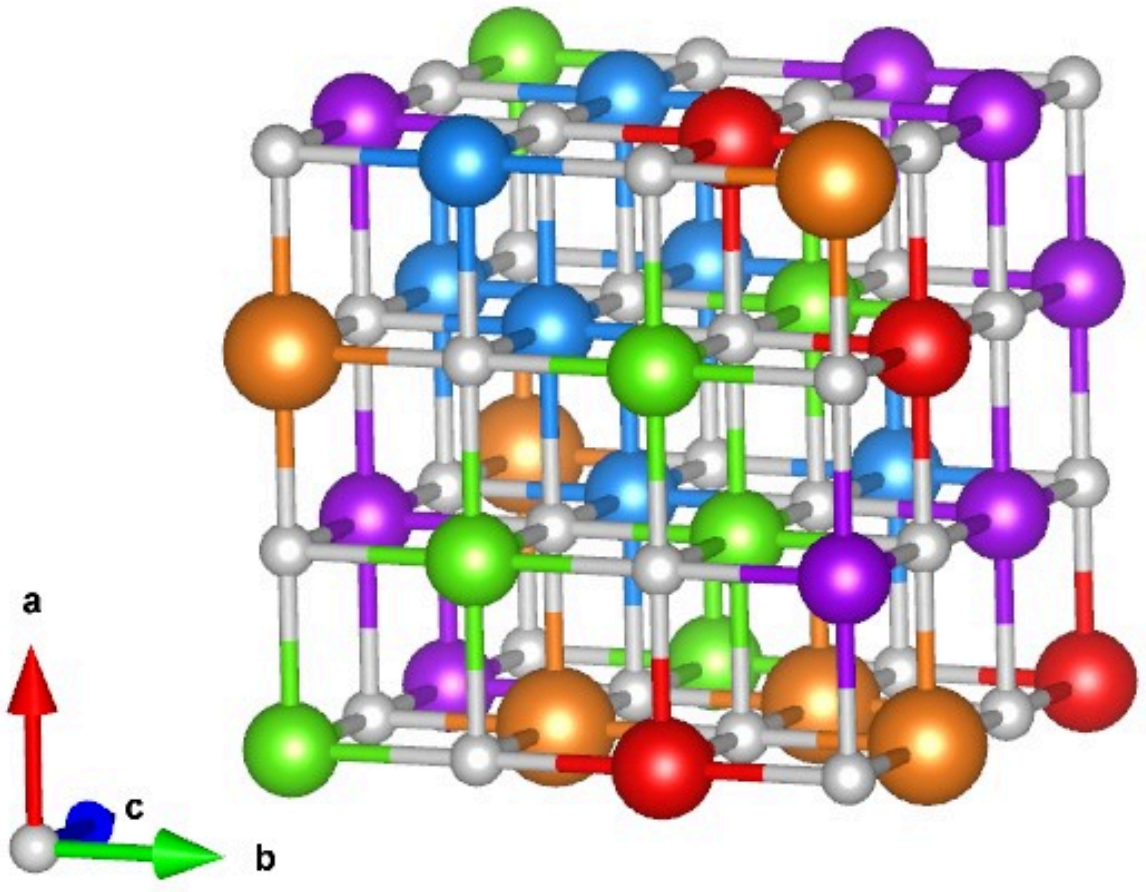

Materials for Energy, Ferroelectrics and Functional Materials

Sb2Te3-Based Organic-Inorganic Thermoelectric Composites

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The move towards more sustainable energy practises in today's world has fuelled the search for alternate and renewable energy sources. Thermoelectric generators (TEG) can generate electricity from heat waste, utilizing resources, that already exist. For example, TEGs can generate electricity from the heat of the human body, which can then be used to power wearable electronics. Inorganic semiconductors have shown the best thermoelectric performance so far – they have higher electrical conductivity and Seebeck coefficient, but also higher thermal conductivity, and moreover, for applications such as wearable electronics, elastic and bendable devices are required. Organic materials offer these advantages and have lower thermal conductivity, but their overall thermoelectric performance is not as effective as inorganic materials. To utilize the best properties of both types of materials, thermoelectric composite systems can be made [1,2].

Antimony telluride is a p-type thermoelectric material that is well suited for room temperature applications and potential for good performance in composite systems. This work employs Sb_2Te_3 nanoparticles with solution processable organic small molecules (OSMs), that are typically used in organic light emitting diodes as charge transport and host materials.

In this work, thermoelectric composite systems of nano and microparticles dispensed in an organic matrix were made using the drop-casting method. The nanoparticles used in this work were synthesized using microwave assisted synthesis. The OSMs were selected from commercially available compounds. Electrical resistance and Seebeck coefficient were measured, and the specific electrical conductivity and power factors were calculated for the samples.

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Keywords

organic small molecules, microwave assisted synthesis, thermoelectric composite systems

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Ferroelectrics and Functional Materials

Dielectric Behavior and Triboelectric Output of TENGs Based on 0.80Na0.5Bi0.5TiO3-0.20BaTiO3/PDMS Composites

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Triboelectric nanogenerators (TENGs), operating through the combined mechanisms of contact electrification and electrostatic induction, enable to convert of low-frequency mechanical energy from ambient motions into usable electrical power [1].

Flexible polymers like polydimethylsiloxane (PDMS) are promising for TENGs due to their strong negative triboelectric polarity and the ability to tune their performance by adding various fillers. The incorporation of various particles into the polymer matrix and the study of their concentration-dependent effects on triboelectric properties have been the subject of numerous research studies [2]. However, comparatively little attention has been devoted to understanding the relationships between microscopic parameters (such as particle size [3], their distribution) and the output performance of TENGs. The solid-solution $0.80Na_{0.5}Bi_{0.5}TiO_3$-$0.20BaTiO_3$ (NBT-20BT) is considered as a filler in a PDMS matrix to partially fill the above-mentioned knowledge gap. The NBT-20BT is a promising lead-free ferroelectric solid solution characterized by enhanced piezoelectric properties and a tunable NBT-xBT composition.

In this study, a series of 14 vol.% NBT-20BT/PDMS-based TENGs with different particle sizes will be prepared using a combination of simple dispersion and spin-coating methods. The NBT-20BT powder will be synthesized via a conventional solid-state reaction method; a subsequent reduction in particle size will be achieved through wet planetary ball milling. The morphology, dielectric behavior as a function of temperature and frequency, and triboelectric output performance of the NBT-20BT/PDMS-based TENGs will be investigated. The effect of NBT-20BT particle size on the relaxation processes and triboelectric properties in NBT-20BT/PDMS system will be analyzed and discussed to reveal potential correlations.

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Keywords

PDMS, Sodium bismuth titanate - barium titanate, Triboelectric nanogenerator, Dielectric properties

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Materials for Energy, Materials for Photonics, Ferroelectrics and Functional Materials

Visible Photoluminescence in Piezoelectric Diphenylalanine Thin Films

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Diphenylalanine (FF) peptide molecules have gained significant attention due to their ability to self-assemble into highly ordered nano/microstructures possessing unique optical and piezoelectric properties [1, 2]. In this work, we developed novel photoluminescent FF thin films by incorporating lanthanide ions (Eu^{3+}) and organic photosensitizers, such as salicylic acid (SA), 1,10-phenanthroline (PHEN), or benzophenone (BZP) during a controlled self-assembly process.

The fabrication followed a specialized two-step mechanism: initially, amorphous FF films were deposited via spin-coating under low humidity (< 30%) to maintain a stable non-crystalline state; subsequently, these films underwent solid-phase crystallization in a climatic chamber at high relative humidity (90%) and elevated temperature (30 °C). During this stage, water vapor-initiated surface nucleation leads to the growth of dense, highly oriented crystalline domains over approximately six hours.

Characterization via luminescence spectroscopy and polarized optical microscopy confirmed that the incorporation of lanthanide ions and photosensitizers leads to the appearance of a significant luminescence signal in the visible range, while maintaining the crystalline film structure important for piezoelectric properties. For example, samples with Eu^{3+} ions incorporated together with PHEN exhibit a strong response in the red region of the spectrum, while samples with SA demonstrate a pronounced response in the blue region. Increasing the concentration of Eu^{3+} ions enables enhancement of the luminescence response up to the limit imposed by film crystallization.

This research successfully demonstrates the possibility of fabricating highly crystalline and photoluminescent piezoelectric FF thin films, offering a promising platform for multifunctional peptide-based optoelectronic devices.

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Keywords

Diphenylalanine, Photoluminescent, Self-assembly, Thin film, Solid-phase crystallization,

Acknowledgements

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Materials for Photonics

Investigation of photochromic films containing Na8Al6Si6O24(Br,S)2

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Hackmanite ($Na_8(Al_6Si_6O_{24})(Cl,S)_2$) is a sulfur-doped sodalite mineral that shows reversible photochromism: it changes color under UV irradiation and returns to its original color when exposed to visible light or when heated. Because of this behavior, hackmanite is a strong candidate for use in photochromic lenses, optical surface coatings, and UV sensors.[1]

In this study, the aim was to identify synthesis conditions that yield the best-performing hackmanite, enhance its photochromic effect, and assess whether the material can be incorporated into photochromic films. Chloride in the lattice was replaced with bromide, and key synthesis parameters, such as reduction temperature and grinding duration were systematically adjusted to maximize the photochromic response. In addition, strategies to reduce particle aggregation during the fabrication of silicone-based photochromic films were tested to produce more homogeneous composites.

Overall, the experiments indicated that increasing color intensity tended to come at the cost of increasing opacity, which set a practical limit on how dark the material could become. As a result, hackmanite may be less suitable for applications requiring high transparency, but it remains well suited for UV sensors and other uses where clarity is not essential. As a proof-of-concept, metameric anti-forgery tagging was also investigated, and the results suggested strong potential for this type of application.

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Keywords

hackmanite, UV sensing, photochromism, tenebrescence

Acknowledgements

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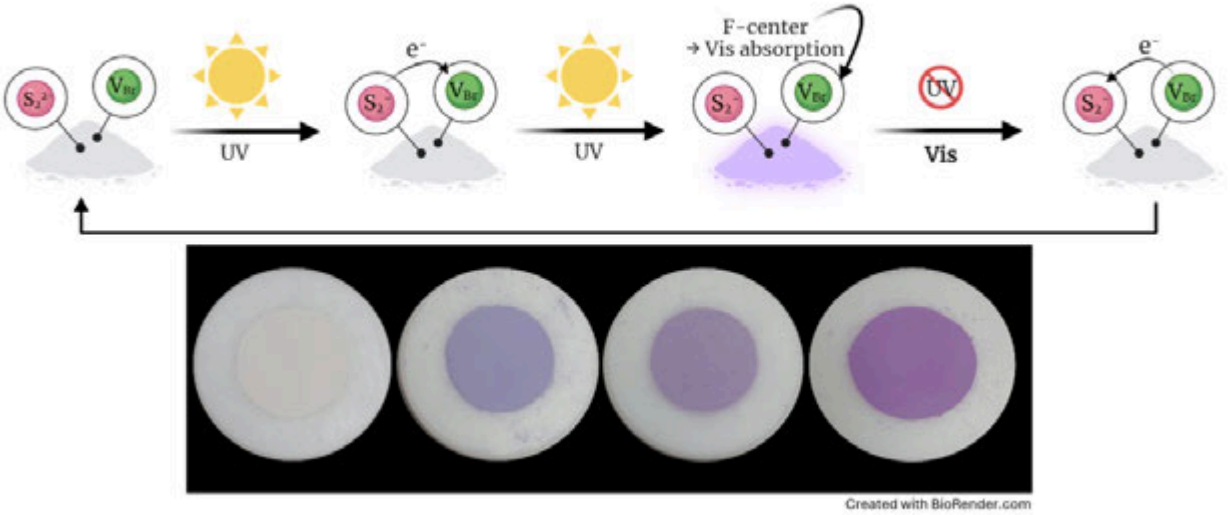
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Ferroelectrics and Functional Materials

Eco-Friendly Terpineol-Based Silver Nanoparticle Ink with Exceptional Stability and High Conductivity for Inkjet Printing

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The increasing demand for low-cost, high-performance printed electronics calls for conductive inks that combine environmental sustainability with reliable jetting and electrical performance. Here we report a novel silver nanoparticle (Ag-NP) ink formulated with terpineol—a biodegradable, low-toxicity solvent—and butylamine as a stabilizer, achieving unprecedented colloidal stability and conductivity for ink-jet applications. Uniform Ag-NPs (< 10 nm) were synthesized via a modified one-pot reduction in the presence of oleic acid and oleylamine, followed by a controlled precipitation/redispersion sequence that replaces long-chain ligands with short-chain butylamine. The resulting ink (13 wt % Ag) exhibits a viscosity of ~10 mPa·s, surface tension of 27 $mN \cdot m^{-1}$, and density ≈1 $g \cdot cm^{-3}$, matching the Dimatix 2850 printer specifications. UV-Vis and DLS measurements confirm that the nanoparticle size distribution remains stable (average hydrodynamic diameter 5–10 nm) over 85 days at room temperature. Inkjet printing of six-layer patterns on glass substrates produces defect-free droplets (≤ 40 µm) with excellent wetting (contact angle 18–21°). Post-printing sintering at 400 °C for 30 min yields continuous silver films with a conductivity of 5.2×10^7 $S \cdot m^{-1}$, corresponding to 81 % of bulk silver. Thermogravimetric and DSC analyses reveal complete removal of organic ligands between 200–400 °C, while XRD and SEM confirm fcc silver crystallinity and grain growth up to 600 nm. The terpineol-based ink thus delivers a rare combination of long-term stability, eco-friendly formulation, and high electrical performance, positioning it as a scalable solution for sustainable printed electronics, RFID antennas, flexible sensors, and other emerging applications [1].

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Keywords

silver nanoparticles, inkjet printing, terpineol, conductive ink, sustainable electronics

Acknowledgements

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Materials for Energy

Enhanced thermovoltage generation in multilayer AAO membranes via interface effects and tunable surface charge

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Efficiently harvesting low-grade thermal energy remains a significant challenge for sustainable energy solutions. Ionic thermoelectric systems using nanoconfined aqueous electrolytes have recently gained interest due to their extremely high thermopower, in which ion transport is strongly influenced by interfacial interactions and surface charge.

Anodic aluminum oxide (AAO) is an environmentally friendly porous material that is beneficial for electrolyte nanoconfinement due to its highly ordered, parallel nanochannel arrays. Its thickness and nanochannel diameters can be precisely controlled, and the inner surfaces can be easily modified by changing the surface charge from positive to negative.

In this study, the multilayer AAO membranes were infiltrated with aqueous electrolytes ($1{\cdot}10^{-4}$ M NaCl and Na_2SO_4) using hydrostatic pressure. The surface charge of the inner AAO nanochannel was adjusted via pretreatment, and its impact on output voltage per Kelvin was demonstrated. Ion transport within the modified nanochannels with electric double layer overlap was studied using electrochemical impedance spectroscopy and cyclic voltammetry. The value of the generated voltage per Kelvin was further enhanced by stacking additional AAO layers, highlighting specific interface phenomena in multilayer structures. The obtained results demonstrate simple strategies to enhance thermovoltage generation and the ionic Seebeck coefficient in nanoconfined aqueous electrolytes.

Keywords

ionic thermoelectrics, nanoconfinement, waste heat, anodic alumina, interface effects

Acknowledgements

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Materials for Photonics, Technologies and Devices

Synthesis of Cu, Ag, and Au Nanoplates for In Situ SEM Studies of Thermal, Electrical, and Plasmonic Heating.

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Silver (Ag), gold (Au), and copper (Cu) nanoplates have attracted significant attention due to their high electrical conductivity and pronounced localized surface plasmon resonance, enabling potential applications in nanoelectronics, plasmonics, and sensing. Understanding their melting behaviour and morphological stability under different excitation modes is essential for reliable device integration. This study focuses on the synthesis of Cu, Au, and Ag nanoplates and their in situ investigation under thermal, current-induced, and laser-induced excitation.

In this work, Au nanoplates are prepared via a chemical reduction self-seeding approach employing hydrogen tetrachloroaurate tetrahydrate, cetyltrimethylammonium bromide, and L-ascorbic acid. Ag nanoplates are synthesized via a self-seeding hydrochemical route using silver nitrate, citric acid, L-ascorbic acid, sodium borohydride, and sodium bis(2-ethylhexyl) sulfosuccinate. Cu nanoplates are synthesized using copper(II) bromide and branched polyethyleneimine, with Ag nanoparticle seeds and L-ascorbic acid as the reducing agent. The obtained materials are characterized by scanning electron microscopy (SEM) to evaluate morphology and size distribution, and by UV–Vis absorption spectroscopy to assess plasmonic bands relevant for excitation studies.

The synthesized Cu, Ag, and Au nanoplates are used in ongoing SEM-based experiments to characterize melting behaviour under three excitation modes: uniform thermal heating, current-induced Joule heating, and laser-induced plasmonic heating. These measurements enable in situ observation of morphology evolution and melting-related transformations. Initial observations indicate differences in transformation kinetics and morphology evolution depending on the excitation mode, and the study is currently ongoing.

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Technologies and Devices

Dual-window photoluminescence gas sensing with ultrathin Eu-doped ZnO films on black aluminium absorbers

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Optical gas sensing based on photoluminescence enables remote, electrically passive readout at room temperature. ZnO defect PL is strongly influenced by surface adsorption and band bending under oxygen and water exposure.[1] Europium provides narrow 4f–4f lines that can be isolated from the broadband host background, and its red emission in ZnO is often defect-mediated.[2] Here we combine ultrathin Eu-doped ZnO (1 at.% Eu; 8–24 nm) films with nanostructured black aluminium (BAl) absorbers, a broadband low-reflectivity coating offering a high-area interface for conformal sensing layers.[3] Under 266 nm excitation at laboratory temperature, the spectra show sharp Eu^{3+} emission superimposed on a broadband background. We define two integrated channels: a Eu window and a broadband window and record dynamic photoluminescence responses (200 ml·min^{-1} flow) during N_2/O_2 switching and humidity steps in synthetic air (50–100% RH). Oxygen/nitrogen exchange reproducibly modulates Eu photoluminescence, whereas humidity produces pronounced quenching that dominates broadband window, indicating spectrally distinct adsorption mechanisms. A temperature regeneration step in N_2 at 150 °C for 80 min increases Eu photoluminescence in most samples, consistent with partial removal of water-related quenchers at the porous BAl/ZnO interface. This dual-window approach enables simultaneous oxygen readout and humidity correction, improving selectivity and mitigating drift under realistic ambient conditions.

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Keywords

Eu doped ZnO, photoluminescence, optical gas sensing, black aluminium

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Materials for Photonics

Nanosecond Laser Processing of Gold Thin Films for Tunable Surface Plasmon Resonance Sensing

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Au nano-island films on ITO/glass substrates were formed by nanosecond laser processing for surface plasmon resonance (SPR) sensing applications. Thin Au films with thicknesses up to 21 nm were restructured into nano-islands using laser-induced dewetting [1]. The morphology of the formed structures depended on the initial film thickness and laser processing parameters. Au nano-islands with equivalent circular diameters between 60 and 420 nm were obtained, affecting the SPR response. A pronounced SPR band near 560 nm was observed for Au nano-islands with intermediate sizes, while very small or large nano-islands showed a weak or absent SPR response. Sensitivity of the SPR signal to changes in the surrounding medium shows potential for sensing applications. Nanoparticle size and interparticle distance were tuned by varying the laser processing parameters. Au nano-island films integrated into hybrid liquid crystal cells enhanced photorefractive effects and accelerated dynamic grating formation with increased nonlinear optical response [2].

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Keywords

nanosecond laser processing, Au nano-islands, surface plasmon resonance, liquid crystals

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Materials for Energy

Characterisation of paramagnetic radiation-induced defect centres in biphasic Li4SiO4-Li2TiO3 ceramics under exposure to various types of ionising radiation

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Tritium breeding using lithium-containing materials is essential to achieve fuel self-sufficiency in nuclear fusion reactors [1]. Understanding the formation and accumulation of radiation-induced defect centres in biphasic Li_4SiO_4-Li_2TiO_3 ceramics under exposure to various types of ionising radiation is crucial for predicting their performance in expected operating conditions. X-rays and accelerated electrons are commonly used in fundamental studies, but neutron irradiation uniquely simulate actual operating conditions by inducing atomic displacements and tritium production via nuclear reactions [2].

In the present work, the formation of paramagnetic radiation-induced defect centres was investigated in biphasic Li_4SiO_4-Li_2TiO_3 ceramics. Solid-state synthesis method was used to prepare the samples for the irradiation experiments (X-rays, accelerated electrons, and neutrons). Prior to irradiation, the chemical and crystalline phase composition was confirmed using various physico-chemical analysis techniques. The irradiated samples were analysed using electron paramagnetic resonance (EPR) spectroscopy.

The EPR spectra of the biphasic Li_4SiO_4-Li_2TiO_3 ceramics after irradiation with X-rays and accelerated electrons exhibited a complex signal structure. The EPR signals with $g \geq 2.00$ correspond to oxygen-related hole centres and E′-type centres, while those with $g < 2.00$ are attributed to titanium-related electron centres. These results will also be directly compared with the EPR spectra of samples irradiated with neutrons.

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Keywords

Lithium ceramics, Ionizing radiation, Radiation-induced defects, Electron paramagnetic resonance spectroscopy

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Materials for Photonics

VUV Luminescence Excitation Spectroscopy of Transition-Metal-Doped YInO3 and Mg4TiO4

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Manganese and chromium ions are important luminescent activators in oxide materials owing to their rich electronic structure and strong sensitivity to the local crystal-field environment. Understanding host-to-activator energy-transfer mechanisms is essential for the rational design and optimization of oxide phosphors. In this context, vacuum-ultraviolet (VUV) excitation spectroscopy is especially informative, since it provides direct access to host-related electronic transitions and their role in the excitation of impurity-related luminescence.

In this work, Mn- and Cr-doped $YInO_3$ and Mg_2TiO_4 were studied by VUV luminescence excitation spectroscopy using synchrotron radiation at the SUPERLUMI experimental station at PETRA III storage ring of DESY [1] and the photoluminescence endstation at the FinEstBeAMS beamline of MAX IV Laboratory [2,3]. Emission was detected in the UV–Vis–IR spectral region at low and room temperatures. The obtained excitation spectra evidence the involvement of fundamental absorption, excitonic excitation, and higher-energy host-lattice electronic transitions in the formation of transition metals related luminescence.

Comparative analysis of the studied oxide materials reveals the role of the host electronic structure and crystal lattice in governing energy-transfer efficiency and luminescence excitation pathways. The results provide new insight into host–activator interactions in Mn-doped oxides and highlight the capabilities of VUV synchrotron spectroscopy for probing excitation mechanisms in transition-metal-activated luminescent materials [4].

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Keywords

luminescence, Mn, VUV, synchrotron radiation, perovskites

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Ferroelectrics and Functional Materials

Tannic Acid–Assisted Design of Ce-Modified CuO with Enhanced Redox Activity

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Tannic acid (TA), a low-cost and environmentally friendly polyphenol, was used to engineer Ce-modified CuO particles through a surface metal–organic coating approach. A TA–Ce layer was deposited onto CuO particles (Figure 1A) and subsequently calcined to obtain Ce-modified CuO composites.

The structural and morphological properties of the materials were investigated using comprehensive physicochemical characterization (XRD, SEM, EDS, DLS, etc.). The oxidative activity was evaluated using the DCFH assay. Compared with pristine CuO, the Ce-modified materials exhibited enhanced oxidative activity in the dark, with approximately twofold higher relative fluorescence intensity after annealing (Figure 1B). According to EDS, the Ce content in the annealed modified CuO was 1.34% ± 0.91 by weight.

This simple and scalable approach provides a promising route for designing redox-active oxide materials with enhanced oxidative functionality.

Figure 1. A) SEM image showing diffuse particle surfaces due to the formation of a TA–Ce coating layer. B) Oxidative activity of CuO-based materials in the dark in deionized (DI) water at concentrations of 10, 100, and 1000 mg/L, expressed as relative fluorescence intensity. The pink line indicates the control (value = 1). Pristine CuO, CuO–Ce with phenolic coating, and CuO–Ce after annealing at 500 °C were compared. Error bars represent the standard deviation of replicate measurements.

Keywords

Ce-modified CuO, redox, catalyst, composite

Acknowledgements

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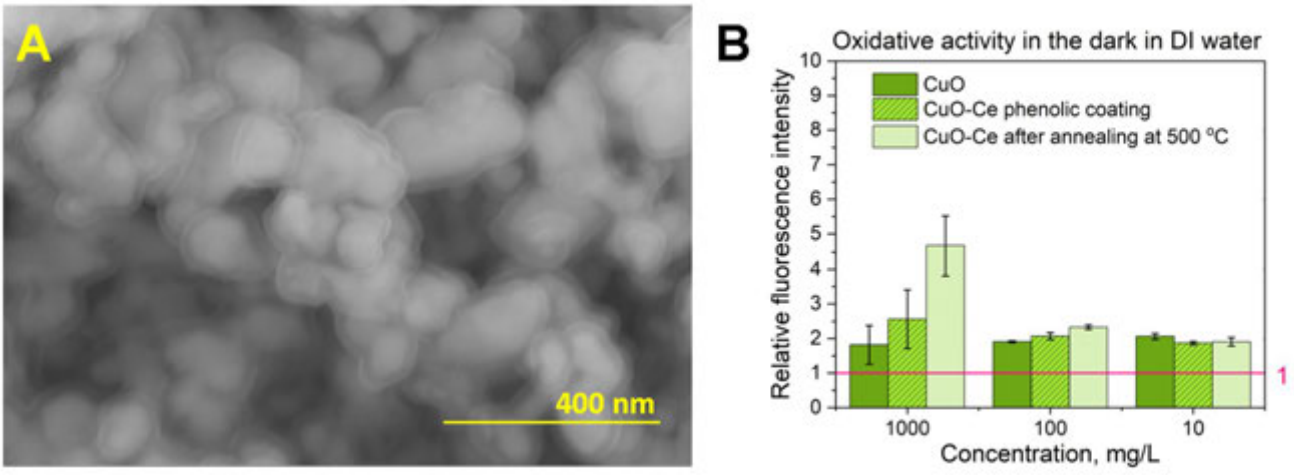
A
400 nm
B
Oxidative activity in the dark in DI water
CuO
CuO-Ce phenolic coating
CuO-Ce after annealing at 500 °C
Relative fluorescence intensity
0
1
2
3
4
5
6
7
8
9
10
1
1000
100
10
Concentration, mg/L

Materials for Photonics, Ferroelectrics and Functional Materials

Effect of DLIP Surface Structuring on Friction Coefficient Under Dry Sliding Conditions

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Laser surface structuring enables precise modification of surfaces, directly influencing tribological performance [1]. Among these techniques, Direct Laser Interference Patterning (DLIP) allows fabrication of regular periodic microstructures with controlled spatial period [2]. In this work, such structures are applied to tailor frictional behavior under dry sliding conditions [3]. The irradiated samples were fabricated from Uddeholm Ramax HH steel, and dry sliding tests were conducted with polyoxymethylene (POM).

DLIP-generated line-like patterns with spatial periods of 2.88–3.05 μm were investigated. Optical microscopy confirmed the formation of periodic structures (Fig. 1) in some processed samples. Tribological testing revealed a significant reduction in the coefficient of friction (CoF) compared to the untreated surface, with the best results observed when both microstructures and oxide layer formation were present. While reference samples exhibited CoF values of ~0.55–0.60, DLIP-structured surfaces reached minimum values of ~0.25, corresponding to a reduction of ~55–60%. The improved performance is attributed to reduced real contact area, debris trapping, and altered stress distribution, demonstrating that DLIP enables controlled friction reduction through tailored surface structuring.

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Keywords

Direct Laser Interference Patterning (DLIP), laser surface structuring, tribology, friction reduction, microstructured surfaces

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Theoretical Modeling of Functional Materials and Devices

DFT-supported ML Design of Mn-Doped BiVO4 Photoanodes for Visible-Light-Driven Water Splitting

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Bismuth vanadate ($BiVO_4$) is a leading visible-light-active oxide photoanode for solar hydrogen production via water splitting due to its suitable band gap, stability, and low cost. However, its photoelectrochemical performance is commonly limited by low charge-carrier mobility and fast electron–hole recombination. In this computational work, we combine density functional theory (DFT) with machine learning (ML)-assisted analysis to evaluate Mn-doped $BiVO_4$ as a tunable material for improved visible-light-driven activity. We quantify how Mn incorporation modifies the electronic structure, including band-gap changes, band-edge alignment relative to water redox potentials, and defect- and distortion-induced states that can influence charge separation. Our DFT results indicate that Mn doping systematically shifts valence- and conduction-band positions and can narrow the band gap compared with pristine $BiVO_4$, extending absorption deeper into the visible region while maintaining energetically feasible redox driving forces. ML analysis of DFT-derived descriptors further identifies Mn concentration, local structural distortion, and band-edge shifts as key predictors of the expected performance, enabling the identification of promising doping windows without exhaustive trial-and-error calculations. These insights are consistent with experimental trends reported for compositionally tuned $BiVO_4$ and $BiVO_4$-based heterostructures, where band engineering and interfacial charge-transfer control improve efficiency. This research has been funded by the Latvian Council of Science grant No. LZP-2024/1-0406.

Keywords

DFT, ML, BiVO4, photocatalysis, hydrogen production

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RIANA – Research Infrastructure Access in NAnoscience & nanotechnology

Toomas Plank , University of Tartu

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Michael Stuckelberger , Deutches Elektronen-Synchrotron DESY, X-Ray Nanoscience and X-Ray Optics

A Horizon-Europe-funded project to assist research in nanoscience and nanotechnology. Coordinated by DESY, the project runs from March 2024 for 4 years. We support curiosity- driven research in nanoscience with open research questions for long-term impact and challenge-driven research in nanotechnology with targeted research questions for short-term and mid-term impact. At the core of the RIANA consortium is the ARIE (Analytical Research Infrastructures in Europe, https://arie-eu.org/) network, which comprises European analytical networks with a focus on large-scale research infrastructures (RIs).

We offer access to the most advanced RIs through a central user office and a single entry point (figure).

Institute of Physics, University of Tartu participates in RIANA network through EuroNanoLab RI. EuroNanoLab is a distributed research infrastructure consisting of 44 state-of-the-art academic nanofabrication centres across Europe.

Keywords

Research Infrastructure, Nanoscience, nanotechnology

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League of European
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Photon Sources


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RADIATE


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EUROPEAN DISTRIBUTED RESEARCH
INFRASTRUCTURE FOR ADVANCED
ELECTRON MICROSCOPY


LENS
LEAGUE OF ADVANCED
EUROPEAN NEUTRON
SOURCES


EUSMI


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Paper production using green algae

Jānis Poots , Riga State german gymnasium

Jānis Poots , Co-researcher
Valters Tolks , Co-researcher

Paper can be made in different ways and from different materials. This paper will describe the making of paper from green algae. The authors of the work aim to introduce an innovative, sustainable paper using only green algae and not creating any harmful by-products. When making paper from seaweed, its original color is based on the type of algae. Chemical bleaching is used to make the paper white, which is the main cause of the chemical by-products, where chemical gasses are released. In the author's work, bleaching is not used, thus preserving nature. The algae were collected on the shores of the Gulf of Riga, and they were washed and dried. The green algae were shredded and boiled in lye for 60 min, 90 min, and 120 min, then they were rinsed with water. In cooperation with the Latvian State Institute of Wood Chemistry, the paper was obtained using a paper-making machine. According to the results, it was concluded that the paper containing algae, which was boiled longer, had the most durability, and this paper outperformed the ordinary woodbased paper in the tensile strength test. A new way of paper production was introduced, which produces minimal chemical by-products.

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Keywords

Kraft, Cellulose, Lignin, Paper, Algae

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Riga State German Grammar School

Paper prouction using green algae

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Supervisor: Daniels Grīnvalds
Consultant: Anda Gromova

Purpose of the work

Process algae according to the established work plan and create paper. Compare the mechanical properties of the created paper with other paper products available on the market.

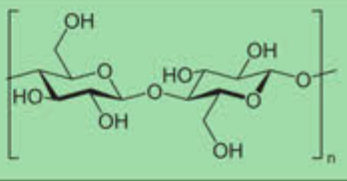
Research hypothesis

It is possible to use green algae to create paper for household or industrial use.

Research methods

1. Literature analysis method
2. Feasibility study method
3. Experimental method
4. Comparative analysis method

Structure of cellulose



Topicality

1. Conservation of wood resources, algea provides an alternative resource for papermaking, this would help protect forests.
2. Washed-up algea produces an unpleasant odor, which ruins the beach going experience. The algea is then removed to less visited places, where it is left to rot.
3. Paper production with algea creates less chemical by-products, the method only uses water and sodium hydroxide.

Properties of green algae

Beneficial for paper production:

- Easy to collect
- Not used industrially
- Lower lignin content
- Quickly renewable
- Widely found
- Disturbing on beaches

Disadvantages for paper production:

- Contains less cellulose
- No specific technologies
- More cleaning needed
- Higher collection weight
- Consume more H_2O
- Not sufficiently studied

Conclusion

Algae is a much more environmentally friendly raw material for paper production; its processing would create fewer environmentally harmful by-products, and its consumption would improve the quality of life of residents.

Mechanical processing of algae

The algae were collected from the shores of the Gulf of Riga, then rinsed with a hose and left in water for **24 hours**, so that the algae would mostly get rid of all unnecessary **organic material**. The green

Photos

Algae mass in the Gulf of Riga.
Source: Images taken by the authors

Boiling algae in NaOH solution.
Source: Images taken by the authors

Dried seaweed, broken into smaller pieces
Source: Images taken by the authors

Paper samples, depending on algea pulp boiling time

60 min

algae were divided by hand into pieces of approximately **15-20 cm** in length and spread on a film in dry conditions, where they were dried until they were completely dry. The algae were then broken into smaller fibers using a blender.

Algae collection from the coast of the Gulf of Riga. Source: Images taken by the authors

Obtaining seaweed paper

The collected, blended algae were boiled with a **5% NaOH** aqueous solution in a ratio of **1:12**. The algae mixture was heated until it reached a temperature of **90°C**. The algae were stirred using a **mechanical stirrer** throughout the process. After boiling, the pulp was rinsed with tap water until it reached a **neutral pH level**, then it was dried in a desiccator for two days.

The next step was the **disintegration** of the dry paper pulp, which was carried out using a special disintegrator. Then the algae mass, together with water, was poured into a **paper machine**, where the algae were agitated to obtain a short suspension. The algae settled on a special sieve, which was then put under pressure. Within 10 minutes, a finished sheet of paper was obtained.

Results

Mechanical properties of seaweed depending on cooking duration

Boiling time [min]	GSM [g/m2]	Paper thickness [µm]	Maximum strength endured [N]	Tensile strength [N/m]	Maximum elongation [%]	Z - TEA [J/m2]
60	56.69	220.9	6.41	640.72	0.77	2.39
90	45.54	186.7	3.54	353.83	0.59	1.41
120	74.84	294.6	13.6	1360.43	0.61	4.01

The result was 10 sheets of paper - one sheet made from algae boiled for 120 minutes, 4 sheets from algae boiled for 90 minutes, and 5 sheets from algae boiled for 60 minutes.

Based on the results obtained, the paper, which was boiled for 120 min, has potential applications in packaging production, for example, in the production of wrapping papers, as well as the paper could be used to create stronger materials, such as corrugated cardboard, which can be used in packaging or construction. When considering the mechanical properties of the resulting paper, the tensile strength stands out the most.

90 min

120 min

Potential and future research

1. The method of papermaking used relies on NaOH, but it works more as a catalyst during the process more than a reagent, this means that potential research could discover ways to reuse the NaOH.
2. By using algea instead of trees, aswell as using less energy, this papermaking method has the potential to save 160 million trees and 312 million tons of CO2 every year, if fully implemented to replace kraft papermaking.
3. This process of papermaking is also cost effective, one A4 page costing around 0,0017 Euros per page.

The hypothesis put forward by the study has been confirmed as the paper was obtained.

1. In the production process, only algae harvested from the beach of Jurmala were used as a source of cellulose.
2. The obtained data on the mechanical properties of paper depend on its thickness, which is influenced by the duration of paper cooking.
3. The paper turned beige as a result, indicating that the process had removed the green pigment without using bleach.
4. The longest-cooked paper can be used industrially because its tensile strength is at a high level.

Materials for Energy

Local Atomic Structure in Entropy-Engineered Thermoelectric Chalcogenides

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Entropy engineering has recently emerged as a promising strategy to enhance thermoelectric (TE) performance by suppressing lattice thermal conductivity through intrinsic atomic disorder while preserving favorable electronic transport [1]. However, the role of local atomic structure in entropy-stabilized chalcogenides remains insufficiently understood.

In this work, we investigate the short-range order and lattice dynamics in a series of cubic multicomponent chalcogenides within the Ag–Sb–Sn–Se–Te system with progressively increasing configurational entropy: $AgSbSe_2$, $AgSnSbSe_3$, and $AgSnSbSe_{1.5}Te_{1.5}$. Temperature-dependent (10–300 K) multi-edge X-ray absorption spectroscopy was employed to probe element-specific local environments. Reverse Monte Carlo modeling [2] of the EXAFS data yielded unified 3D structural models consistent with all absorption edges.

The extracted element-resolved partial pair distribution functions and mean-square displacement parameters allow separation of thermal and static disorder contributions. Despite the cubic average structure, the local analysis reveals a splitting of Sb–Se bond distances consistent with off-center displacement of Sb atoms from their ideal octahedral positions.

The results provide experimental insight into local lattice distortions and their evolution with increasing configurational entropy, clarifying their role in phonon scattering in TE materials.

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Keywords

EXAFS, thermoelectric, reverse Monte Carlo, configurational entropy

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Materials for Photonics

Ni-DABT and Mo-DABT Coordination Polymers for Flexible X Ray Detectors

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Coordination polymers based on transition-metal DABT (diaminobenzothiazole) linkers offer promising opportunities for flexible radiation-sensing materials. In this study, we report the synthesis and characterization of two DABT-based coordination polymers, Ni-DABT and Mo-DABT, developed for flexible X-ray detector applications. X-ray diffraction confirmed the formation of crystalline coordination networks. Optical absorption spectroscopy revealed broad metal–ligand charge-transfer features, while X-ray absorption spectroscopy provided insights into the local coordination environment and oxidation states of Ni and Mo.

Thin films of Ni-DABT and Mo-DABT were fabricated on flexible substrates using solution-based deposition. Electrical measurements demonstrated stable semiconducting behavior with uniform film morphology. Both materials exhibited a distinct X-ray-induced photocurrent response, showing reproducible switching and sensitivity under irradiation. These results highlight the potential of DABT-based coordination polymers for next-generation flexible X-ray sensing technologies.

Keywords

Ni-DABT, Mo-DABT, X Ray Detectors

Acknowledgements

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Materials for Photonics, Technologies and Devices

Ce3+-activated materials for optical temperature sensors in 0 °C – 400 °C range

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The operation of traditional temperature sensors, such as thermocouples and thermoresistive sensors, can be significantly compromised in electromagnetic fields and aggressive environments. To overcome these limitations, optical temperature sensors are utilised. This study examines the properties of Ce^{3+} activated materials for potential application in optical temperature sensors.

The analysed materials exhibit Ce^{3+} photoluminescence when excited by 450 nm laser light, producing an emission peak at approximately 550 nm. The luminescence decay times characteristic of Ce^{3+} ions are in the range of a few tens of nanoseconds and were measured using a high-speed measuring device. For the studied materials, temperature-induced variations in luminescence decay times associated with thermal quenching occur over different temperature intervals within the range of 0 °C – 400 °C. An overview of temperature-dependent luminescence lifetimes in various materials has been compiled for future applications.

Keywords

Sensors, Optical materials, Photonics

Acknowledgements

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Ferroelectrics and Functional Materials

Surface Functionalization-Driven Control of Magnetic Characteristics in $CoFe_2O_4$ Nanoparticles

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Magnetic nanoparticles exhibit tunable size-dependent physicochemical and magnetic properties, making them attractive for applications in data storage, magneto-optical devices, photocatalysis, and biomedicine [1,2,6]. Cobalt ferrite ($CoFe_2O_4$) is a technologically important ferrite due to its high magnetocrystalline anisotropy, chemical stability, and mechanical hardness. However, its structural and magnetic properties are strongly governed by particle size, morphology, and surface chemistry, which are highly sensitive to synthesis conditions. Established synthesis routes such as hydrothermal, sol-gel, and co-precipitation methods enable modulation of nucleation and growth kinetics through parameters including temperature, pH, and stirring rate [3,4,5]. Despite these advantages, $CoFe_2O_4$ nanoparticles typically exhibit strong agglomeration arising from high surface energy and magnetic dipole interactions, which limits their functional performance. Surface modification using surfactants or capping molecules has been shown to mitigate aggregation through electrostatic and steric stabilization while enabling controlled particle growth and surface functionalization [6].

Herein, $CoFe_2O_4$ nanoparticles were synthesized via a hydrothermal co-precipitation route in the presence and absence of amino acids acting as capping agents [1,7]. We systematically examined the role of amino acid functionalization on the crystallographic structure, morphology, and magnetic behavior using XRD, TEM, VSM, BET analysis, and UV spectrometry. These findings suggest that amino acid-modified $CoFe_2O_4$ nanoparticles are promising candidates for magnetically recoverable adsorbents and catalytic systems in wastewater treatment.

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Keywords

Nanomaterials, Magnetic nanoparticles, Ferrites, Adsorption, Environmental remediation

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Materials for Photonics

Enhanced Mn2+ luminescence in Ti4+ co-doped calcium hexaaluminate

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In recent years, Mn^{2+} has attracted considerable attention as an activator in luminescent materials due to its natural abundance and low cost. Mn^{2+}-activated phosphors are promising candidates for display and solid-state lighting applications. Beyond display technologies, Mn^{2+}-doped phosphors have also demonstrated significant potential in emerging applications, including optical temperature and pressure sensing, as well as persistent luminescent materials for anti-counterfeiting. However, stabilizing Mn^{2+} in oxide lattices synthesized under oxidative conditions remains a major challenge because manganese tends to oxidize to Mn^{3+} and Mn^{4+}. In this work, a Ti^{4+} co-doping strategy was employed to control the oxidation state of manganese in $CaAl_{12}O_{19}$ synthesized in air. Mn-doped $CaAl_{12}O_{19}$ exhibits green emission at 518 nm attributed to Mn^{2+} and red emission at 656 nm assigned Mn^{4+}. To regulate the valence state of manganese, $CaAl_{12}O_{19}$:Mn phosphors were co-doped with varying concentrations of Ti^{4+}. The coupled substitution of Mn^{2+} and Ti^{4+} effectively suppresses the formation of Mn^{3+} and Mn^{4+} while promoting the formation of Mn^{2+}. The enhanced luminescence performance is mainly attributed to the diminished non-radiative energy transfer from Mn^{2+} to Mn^{3+}/Mn^{4+}, as well as increased concentration of Mn^{2+}. An optimized composition achieved a maximum absolute photoluminescence quantum yield of 64.9% for Mn^{2+} emission.

Keywords

calcium aluminate, manganese, luminescence, co-doping, optical materials

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Theoretical Modeling of Functional Materials and Devices

MLIP Factory: An End-to-End, Ab-Initio-to-GPU Workflow for Radiation Damage in Complex Ionic Compounds

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We present a machine-learning interatomic potential (MLIP) study of radiation-induced defect cascades in barium fluoride (BaF_2) and an end-to-end pipeline for building q-SNAP-style MLIPs applicable to multicomponent materials. Our hybrid MLIP combines long-range Coulomb interactions (PPPM in LAMMPS), a short-range q-SNAP[1] term, and a Ziegler-Biersack-Littmark (ZBL) short-range correction. The pipeline centers on on-the-fly enrichment of the training set with diverse MD-sampled configurations (equilibrium, strained, defected, collision-like), using structures up to ≈100 atoms to balance cost and local-environment diversity. Reference data for BaF_2 were obtained from hybrid-DFT (HSEsol) calculations with CRYSTAL23; during training the MLIP's forces, energies, and stresses consistently agreed with DFT. Cascade MD employed PKAs along multiple directions with thermostatted NVT boundaries and an unconstrained NVE core; defects were analyzed after relaxation. The workflow scales to 10^5-10^6 atoms and exhibits substantial wall-time acceleration on modern GPUs, enabling large, accurate MD studies of irradiation effects. We also built a q-SNAP potential for the ternary spinel $MgAl_2O_4$, demonstrating applicability to three-element and other complex chemistries.

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Keywords

qSNAP, MLIP, RADIATION CASCADE, MACHINE LEARNING

Acknowledgements

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Materials for Photonics, Theoretical Modeling of Functional Materials and Devices

First principles study of Mg2TiO4 inverse spinel: Critical comparison of pure and Mn4+ doped materials

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Mg_2TiO_4 (MTO) doped with Mn^{4+} (Mn instead of Ti) is a promising material for production light-emitting diodes (LEDs). MTO is an inverse spinel in which Ti^{4+} and Mg^{2+} ions in a 1:1 ratio occupy octahedral sites, and only Mg^{2+} ions occupy tetrahedral sites. MTO exists in two modifications: high-temperature (cubic space group 227, *Fd-3m*) and low-temperature (tetragonal space group 91, $P4_122$) [1]. The structural transition between phases occurs at a temperature about 700°C. The tetragonal phase is considered as completely ordered form, where Ti^{4+} and Mg^{2+} ions in octahedral sites are located in different Wyckoff positions (4b and 4a, respectively). In this phase, crystallographic unit cell of MTO contains 8 Mg, 4 Ti and 16 oxygen atoms (4 formula units). Opposite, the cubic phase is disordered. It is characterized by a statistical distribution of Mg^{2+} and Ti^{4+} cations in octahedral sites. These cations randomly located in a single Wyckoff positions (16d). Crystallographic cell in cubic phase contains 8 formula units (56 atoms).

In this study, first principles simulations of pure MTO and MTO:Mn^{4+} were performed within the linear combination of atomic orbitals (LCAO) approximation of the density functional theory (DFT), as implemented in CRYSTAL23 computer code [2]. Two possible spin configurations of Mn^{4+} ion in MTO were considered in the framework of the unrestricted (open shell) DFT-LCAO calculations. The structural, electronic, vibrational, dielectric and elastic properties of materials were investigated, compared and discussed.

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Keywords

Mg2TiO4, inverse spinel, dopant, phosphors, first principles DFT-LCAO calculations

Acknowledgements

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Materials for Photonics

Radiometric evaluation of persistent phosphors: Towards reliable power density measurements

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Persistent phosphors are widely investigated for applications ranging from safety markings to medicine. Despite extensive research, emission performance is frequently reported using relative intensities that are dependent on the sensitivity and configuration of the signal detection system. Reliable and reproducible comparison between the emission intensity of different phosphors is therefore essential for meaningful evaluation of persistent phosphor performance and their practical applications [1].

In this work, methodological aspects of radiometric power density estimation for persistent phosphors are investigated. Si-extended photodiode measurements acquired over a small solid angle are used to estimate the radiance of persistent luminescence phosphors after excitation. Experimental parameters that may influence the reliability of the method, including detection geometry, angular emission characteristics and the spectral responsivity of the detection system are analysed. $SrAl_2O_4$: Eu^{2+}, Dy^{3+} and $Sr_2P_2O_7$:Pr^{3+} are used as model persistent phosphor materials to illustrate the methodological approach. The results highlight practical factors influencing radiometric power density evaluation and aim to contribute towards more reliable quantitative characterization of persistent luminescence materials.

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Keywords

Persistent Luminescence, Radiance, Methodology, Phosphate, Stronitum Aluminate

Acknowledgements

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Theoretical Modeling of Functional Materials and Devices

Data-Driven Calibration of LED Illumination Angles in Fourier Ptychographic Microscopy

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Precise knowledge of illumination geometry is critical for accurate quantitative phase reconstruction in Fourier Ptychographic Microscopy (FPM), a computational imaging technique increasingly employed for high-resolution characterization of micro- and nanostructured materials at mesoscale. In practical implementations, the actual illumination angles produced by LED arrays frequently deviate from their nominal design values due to mechanical tolerances, positional errors, and optical misalignment. Such deviations introduce systematic reconstruction artifacts that degrade both amplitude and phase accuracy.

We propose a data-driven self-calibration method for estimating the true illumination angles directly from experimentally acquired image data without the need for dedicated calibration targets or hardware modifications. The method operates in Fourier space, where brightfield images exhibit circular pupil boundaries whose displacement encodes the illumination direction. Illumination parameters are determined through a structured polar-coordinate circle-fitting procedure combined with Gaussian pre-filtering to enhance robustness against noise.

A weighted outlier-rejection scheme based on rigid geometric transformation ensures global consistency of the illumination model and enables extrapolation of the calibration to dark field images. Experimental validation demonstrates improved reconstruction fidelity and phase accuracy in FPM imaging.

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Regina Eckert, Zachary F. Phillips, and Laura Waller, "Efficient illumination angle self-calibration in Fourier ptychography," Appl. Opt. 57, 5434-5442 (2018)

Keywords

Ptychography, Fourier optics, Microscopy, Nanostructures, Metrology

Acknowledgements

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Microfluidics and Biomedical technologies

PANI–MXene Nanocomposite Modified Electrodes for Electrochemical Glucose Biosensing

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The increasing prevalence of diabetes continues to drive the development of reliable electrochemical biosensors for glucose monitoring [1, 2]. Improving the electrode surface remains one of the key approaches to enhancing biosensor performance, particularly in systems based on enzyme immobilization and amperometric detection. MXenes have become an important class of two-dimensional functional materials due to their high electrical conductivity, tunable surface chemistry, and suitability for solution-based processing [3, 4]. Their combination with conducting polymers offers a promising strategy for creating nanocomposite interfaces with improved charge-transfer properties and a favorable surface environment for enzymatic sensing [5].

The main aim of this study was to develop an electrochemical glucose biosensor based on a glassy carbon electrode modified with a polyaniline (PANI)–MXenes nanocomposite. PANI and $Ti_3C_2T_x$ MXenes were synthesized separately and characterized using scanning electron microscopy and UV–Vis spectroscopy to evaluate their morphological and optical features. The modified electrode was used as a functional interface for glucose oxidase immobilization and glucose detection.

The PANI–MXenes modified electrode showed stable and reproducible amperometric responses to glucose, indicating effective electron transfer and retained enzymatic activity. These results demonstrate the potential of PANI–MXene nanocomposites as functional materials for enzymatic glucose biosensors.

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Keywords

biosensors, MXenes, MXenes-PANI, glucose biosensors, glucose oxidase

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Technologies and Devices

Frequency-Domain Optical Temperature Sensing Using Mn^{2+}/Mn^{4+} Luminescence Decay Kinetics in Aluminate Phosphors

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Optical temperature sensing is attractive for applications where electrical probes or direct-contact sensors are unsuitable, such as chemically aggressive, electrically sensitive, or physically inaccessible environments. In this study, a fibre-compatible sensing concept is developed for wide-range temperature measurements, covering approximately - 150 °C to +350 °C. The method relies on manganese-doped complex aluminate phosphors and uses frequency-domain detection of luminescence decay, so that temperature is evaluated from the phase delay between the modulated excitation and emitted light.

The sensing materials were prepared as polycrystalline strontium magnesium aluminates containing either Mn^{2+} or Mn^{4+} emission centres. Optical characterization under blue-light excitation showed two well-separated spectral responses: green Mn^{2+} emission with a maximum at about 525 nm and red Mn^{4+} emission centred near 687 nm. This separation allows the two signals to be analysed independently and combined in a dual-channel thermometric scheme.

Phase-sensitive measurements were carried out with sinusoidally modulated excitation in the 10-150 Hz range. The two manganese centres exhibited different but complementary thermal behaviour. The Mn^{4+}-based red channel provides stronger response at lower temperatures, while the Mn^{2+}-based green channel is better suited for higher-temperature operation. The obtained phase sensitivities, reaching approximately 0.08 deg/K for Mn^{4+} and 0.1 deg/K for Mn^{2+}, indicate that combining both emission centres can broaden the usable measurement range and support continuous all-optical temperature readout from cryogenic to elevated temperatures.

Keywords

sensors, luminescence, transition metals

Acknowledgements

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Materials for Energy

FLEXIBLE CNT-CHALCOGENIDE HYBRID STRUCTURES FOR SCALABLE THERMOELECTRIC ENERGY HARVESTING

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The growing demand for sustainable and maintenance-free energy sources has accelerated research on flexible thermoelectric generators (FTEGs) for converting waste heat into electrical energy. Such systems are particularly relevant for wearable electronics and low-power devices [1].

In this work, flexible hybrid thermoelectric structures based on multi-walled carbon nanotube (MWCNT) networks integrated with inorganic chalcogenide materials are developed and systematically investigated. The hybrid films consist of CNT-Bi_2Se_3 (n-type) and CNT-Sb_2Te_3 (p-type) networks were fabricated on a Kapton substrate via CNT spray followed by sequential physical vapour deposition of chalcogenide layers using shadow masking. To further improve durability, the fabricated networks were encapsulated within a polymer matrix [2,3] in a novel zebra-like multi-leg p-n architecture.

Structural characterization using scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDX) confirmed the formation of uniform and interconnected hybrid networks. Electrical measurements exhibited linear current-voltage characteristics, indicating ohmic behaviour and stable charge transport. Thermoelectric measurements demonstrated enhanced output voltage with the multi-leg architecture outperforming simpler configurations. These results highlight the potential of zebra-like multi-leg CNT-chalcogenide-based hybrid structures for scalable and flexible energy harvesting near room temperature.

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Keywords

Flexible thermoelectric generator; Multi-walled carbon nanotubes (MWCNTs),

Acknowledgements

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Ferroelectrics and Functional Materials

Enhanced Dark Redox Activity of CuO/CeO_2 Composites

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CuO/CeO_2 p–n heterojunction composites have been widely investigated as photocatalysts under UV, visible, or solar light. However, their catalytic behavior under purely dark conditions remains largely unexplored. [1,2] In this work, redox-active CuO/CeO_2 composites with catalytic activity in the absence of light were developed using a modified precipitation synthesis enabling tunable redox activity.

The materials were characterized using a range of physicochemical techniques (XRD, SEM, EDS, DLS, etc.) to elucidate their structural and surface properties. The redox functionality of the composites was evaluated using the DCFH assay; the highest relative fluorescence intensity of the CuO/CeO_2 composites exceeded that of pristine CuO by more than a factor of 25 after 2 h and remained high even after 24 h (Figure 1), indicating pronounced oxidative activity and strong surface redox reactivity under dark conditions.

The practical relevance of redox modulation was further demonstrated by catalytic degradation of model organic dyes (Direct Red and Indigo Carmine), supported by reactive oxygen species (ROS) scavenging experiments and desorption tests, and antibacterial activity. These results highlight the potential of CuO/CeO_2 composites as dark redox-active catalysts for environmental applications.

Figure 1. Oxidative activity of CuO/CeO_2 composite in the dark in deionized (DI) water at concentrations of 10, 100, and 1000 mg/L, expressed as relative fluorescence intensity (2h and 24h). The pink line indicates the control (value = 1). Pristine CuO and CuO/CeO_2. Error bars represent the standard deviation of replicate measurements.

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Keywords

CuO/CeO2, redox, catalyst, composite

Acknowledgements

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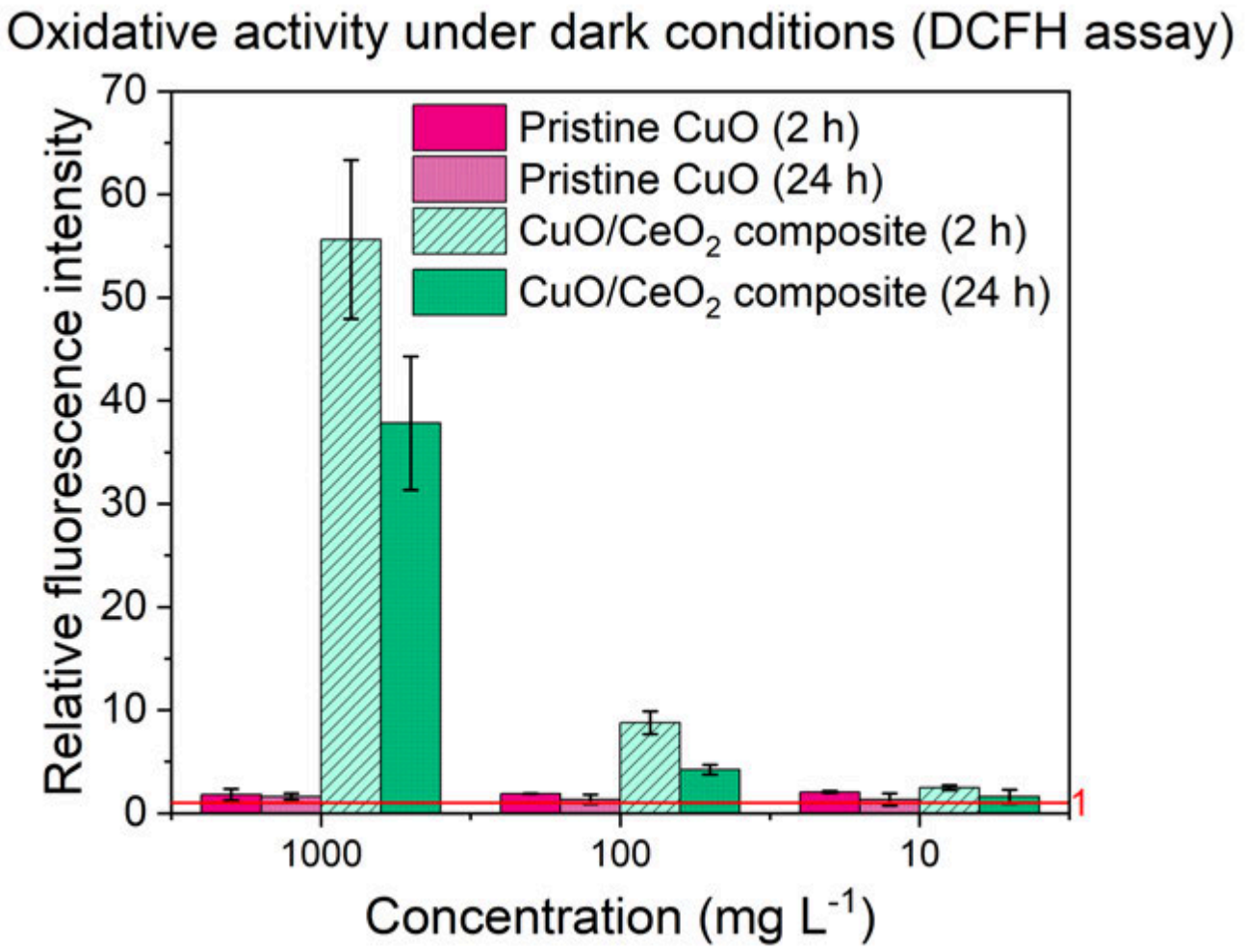

Materials for Photonics

Optical absorption of interstitial oxygen in silicon dioxide.

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Silicon dioxide, in particular in its glassy form is the most-used oxide material in high-power and UV optics, optical communications, microelectronics and nanotechnologies. Radiation-induced point defects are detrimental for SiO_2-based devices. The basic defect, the oxygen vacancy, shows a strong absorption band with peak in vacuum UV (ħw=7.6 eV), well-studied by numerous experimental and theoretic studies. In contrast, the optical absorption of the complementary defect, an interstitial oxygen atom, is experimentally still not established. In irradiated glassy SiO_2, O-vacancies are formed. The ejected oxygens undergo dimerization, forming interstitial O_2 molecules, well-detected by their luminescence. In contrast, O_2 is not formed in α-quartz [1]. In this case the interstitial O associates with a normal O in quartz lattice, forming Si-O-O-Si bond (“peroxy linkage”, POL). This has been predicted by numerous calculations (e.g., [2-4]). Several optical absorption transitions of low oscillator strength (10^{-2}-10^{-3}) are predicted in the 5-7 eV spectral region [3,4]. However, experimental data on POL absorption in SiO_2 is lacking up to now.

We report VUV absorption spectra of high purity α-quartz irradiated by 2.5 MeV electrons up to doses of 2.5 – 3.5 GGy. Apart from an intense (>100 cm^{-1}) O vacancy band at 7.6 eV, weak bands in the 6.4-7.2 eV region were induced. EPR and photoluminescence studies show that they are not related to O or Si dangling bonds. Finally, their correlation to the 7.6 eV band intensity indicates that they can be assigned to POL in quartz lattice. Similar POL centers are expected as well in glassy SiO_2, however, their weak optical absorption is masked by absorption of radiation-induced O_2 molecules.

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Keywords

silicon dioxide, radiation, oxygen defects

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Theoretical Modeling of Functional Materials and Devices

Interpretation of EXAFS spectra of CeO2 using MACE, NequIP, and CHGNet Foundational Models

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Modelling EXAFS spectra with accurate inclusion of thermal disorder effects remains challenging. Molecular dynamics (MD) simulations can be used to calculate distributions of atoms at different temperatures and compare resulting spectra with the experiment, however accurate first-principles MD simulations are computationally expensive. Universal machine learning interatomic potentials (uMLIPs) allow to accelerate first-principles MD, boosting analysis and interpretation of experimental EXAFS spectra. This work investigates accuracy of EXAFS spectra obtained from MD performed with uMLIP foundational models MACE-MPA-0, MACE-MP-0b3 [1], NequIP-OAM-L [2] and CHGNet [3] at 20 and 500 \degree C temperatures with CeO_2 (ceria) as a model system.

Modelling ceria EXAFS spectra is particularly difficult, because of the presence of double excitation peaks and additional peaks due to mixed-valence states (4f0 and 4f1L final configurations)[4]. While double excitation peaks are ignored in this work, mixed valence effect has been successfully approximated by additional post-modelling procedure that accounts for splitting between the two states. All models reproduce spectra well, with MACE-MPA-0 performing best for 20 \degree C and NequIP-OAM-L for 500 \degree C. CHGNet has reproduced spectra slightly worse than other models, but the agreement with experiment has been improved after fine-tuning CHGNet on first-principles data.

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Keywords

uMLIP, molecular dynamics, MACE, NequIP, CHGNet, CeO2

Acknowledgements

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Ferroelectrics and Functional Materials

Hydrogen partial pressure as a key parameter in the reactive sputtering of photochromic YHO thin films

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Oxygen-containing yttrium hydride (YHO) thin films have attracted considerable interest as smart materials due to their reversible photochromic response [1]. Although the effects of parameters such as sputtering pressure and film thickness have been studied [2], the influence of the H_2 partial pressure during sputtering on crystallographic texture and photochromic performance is still not fully understood.

In this study, YHO thin films were deposited by reactive pulsed-DC magnetron sputtering under varying H_2/Ar flow ratios to investigate how the sputtering atmosphere influences YHO structural and optical properties.

XRD revealed a strong dependence of crystallographic texture on the H_2/Ar ratio: highly <100>-textured films formed at low H_2/Ar ratios progressively evolved into more polycrystalline microstructures with slightly reduced crystallite size as the hydrogen content increased. The optical transmittance gradually decreased from approximately 85 % to 70 % as the H_2/Ar ratio was raised to 0.6, followed by a sharp drop at higher hydrogen contents. The photochromic contrast of 690–820 nm thick YHO films decreased from 14 % to 7 % as the H_2/Ar ratio increased from 0.08 to 0.60. Thinner films (360–490 nm) exhibited a similar but less pronounced trend. Bleaching kinetics indicated faster recovery, with effective bleaching time constants of approximately 1–15 min for films deposited at H_2/Ar < 0.25. XPS revealed higher oxygen incorporation in films deposited at lower H_2/Ar ratios, deviating from the commonly reported correlation between oxygen content and photochromic response in YHO.

These results demonstrate that low H_2 partial pressure during reactive sputtering is advantageous for achieving higher optical transparency, enhanced photochromic contrast, and faster bleaching kinetics in YHO thin films.

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Keywords

photochromism, oxygen-containing yttrium hydride (YHO), H2 partial pressure, thin films, reactive magnetron sputtering

Acknowledgements

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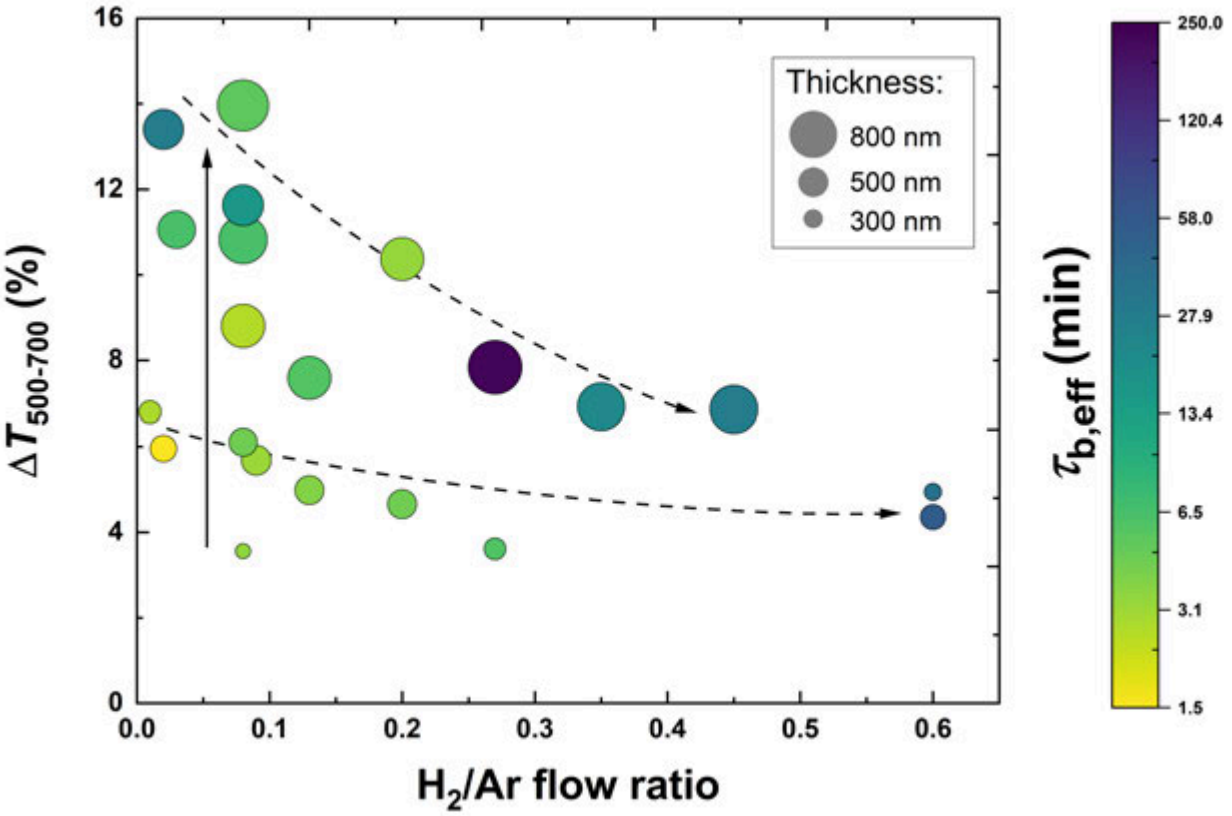

Microfluidics and Biomedical technologies

Specificity analysis of the GreenB1 aptamer in pancreatic ductal adenocarcinoma models: a comparative study of static and microfluidic environments

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GreenB1 is an integrin β1 (ITGB1) specific aptamer, and assessing its specificity on PDAC cell lines, organoids, and organ-on-chip (OoC) model systems would provide in-depth information about the GreenB1 aptamer's ability to bind to tumour cells, depending on environmental conditions. The aim of the current study was to characterise the affinity of GreenB1 under static and microfluidic conditions. To achieve this, experimental condition optimisation and GreenB1 affinity testing were performed using ImagestreamX MarkII (Cytek Biosciences) imaging flow cytometer (FC). OoC model systems with and without endothelial channels were established using 4-channel CellBox Labs microfluidic chips. GreenB1 binding validation in microfluidic conditions was assessed using immuneluorescence analysis (IF). The fluorescence signal of GreenB1 was amplified with Alexa Fluor^{TM} 488 Tyramide SuperBoostTM kit. The resulting FC data indicate that Capan cells have a superior affinity for GreenB1, and they were further used in an OoC system. Signal amplification enabled the visualisation of aptamer binding to Capan cells in a PDAC OoC model. GreenB1 binding conditions were optimised for the Capan cell line to be further used in the OoC system. Preliminary data demonstrate that GreenB1 binding is detectable in an OoC system. These findings support the feasibility of developing a further aptamer-based targeted delivery approach in physiologically relevant conditions.

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Keywords

Aptamers, Microfluidics, PDAC

Acknowledgements

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Materials for Photonics

Tuning the Luminescence Properties of Hackmanite with Zinc

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Both natural and synthetic hackmanites [$Na_8(AlSiO_4)_6(Cl,S)_2$] are known to have diverse luminescence properties, such as bluish white and orange emission, and white persistent luminescence. When synthesising hackmanites, it is possible to modify these properties via ion doping and structural changes by ion exchange.

Previous studies have shown that multiple ions in hackmanite structure have been successfully changed with new ones (e.g. Ca, Ga, and Ge), and the optical properties have changed. However, these studies have focused on the photochromic properties instead of luminescent ones. In this study, some of the Na^+ ions have been changed with Zn^{2+} ions in hackmanite structure. The material was synthesised via high temperature solid-state reaction, and the characterisation was done with X-ray powder diffraction (XRPD), which conducted that the product is a mixture of hackmanite, NaCl, Zn_2SiO_4, and ZnS being the significant phases.

This zinc hackmanite has new luminescence properties, including 230 nm excited UV and red emission, 330 nm excited blue-green emission, and green afterglow that can be excited with visible light. Based on SEM-EDX combined with cathodoluminescence, it is possible, that the ZnS phase is responsible for the blue-green emission and green afterglow. The red/near-infrared emission could be due to Fe^{3+} impurities in hackmanite structure. The UV emission (λ_{em}=375 nm) could be due to Ti^{4+} impurities, but it needs to be studied more to be understood better.

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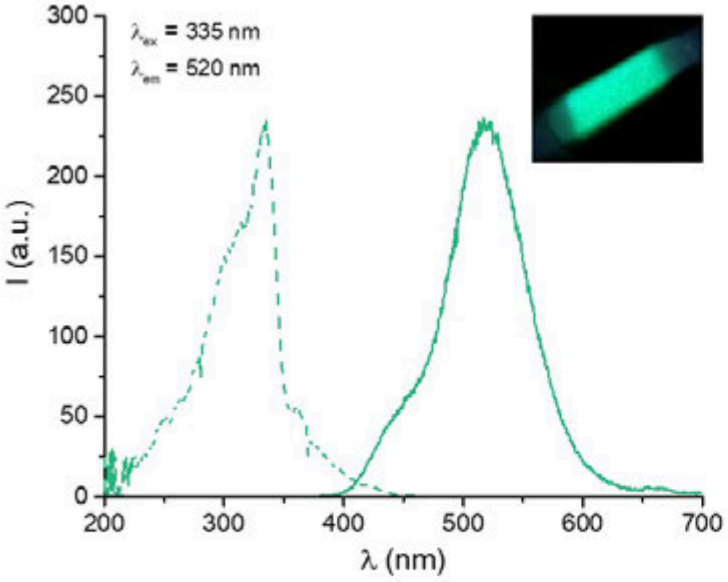
Keywords

Hackmanite, Luminescence, Zinc

Acknowledgements

Jane and Aatos Erkko foundation is acknowledged for funding. The Materials Research Infrastructure (MARI) at University of Turku, is acknowledged for access and support with the SEM and XPS facilities.



Materials for Photonics

Excitation and relaxation of bound excitons in Cu2O single crystal and thin film

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Excitation and relaxation processes of photoluminescence (PL) from bound excitons were studied in Cu_2O single crystal [1] and Cu_2O thin films electrodeposited on copper substrate [2] under irradiation of the wavelength-tunable laser in the 10-300 K temperature range. For both types of samples PL emission bands at 1.72 eV, 1.53 eV and 1.36 eV were observed and assigned to bound excitons localized at oxygen and copper vacancies V_O^{2+}, V_O^{+}, V_{Cu}, correspondingly. Photoluminescence excitation (PLE) covers the violet, blue, green and yellow exciton region (2.9 -1.8 eV) and a red band (1.93 eV) assigned to the direct excitation of oxygen-vacancy-bound exciton. For both types of Cu_2O samples PL thermal decay curves have a non-monotonous character with signs of negative thermal quenching implying a complex process of bound exciton relaxation. The shape of PL and PLE spectra and mutual ratio of subbands as well as features of luminescence activation energy are specific for each type of Cu_2O. The observed difference in PL and PLE spectra of Cu_2O thin films from those of Cu_2O single crystal are explained by the higher concentration of structural defects, such as grain boundaries, dislocations, interface and surface defects, causing broadening, diminishing and shifting of particular emission bands. Numerous defects, both radiative and non-radiative, produce additional trapping centres for bound excitons, influencing the processes of bound exciton thermal relaxation.

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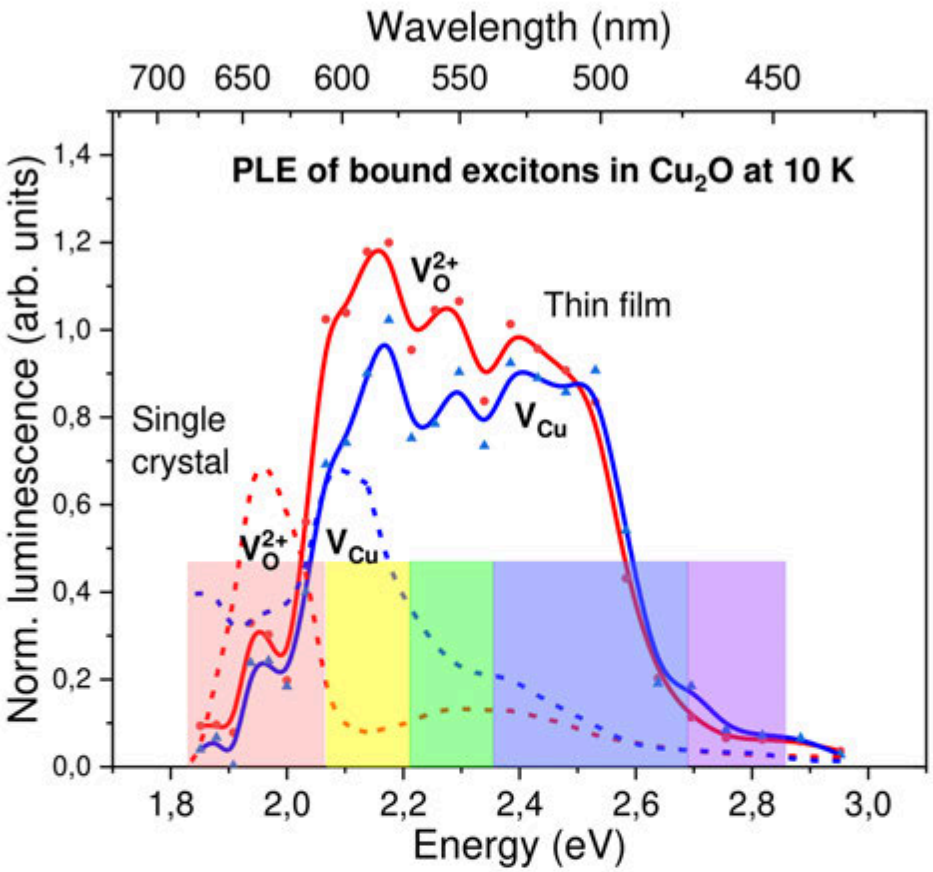
Keywords

cuprous oxide, bound exciton, photoluminescence, excitation, relaxation

Acknowledgements

The work was supported by funding from the Taiwan and the Baltic States Research Center on Physics at the Institute of Solid State Physics, University of Latvia, Riga, Latvia.


Wavelength (nm)
700 650 600 550 500 450
PLE of bound excitons in Cu2O at 10 K
Norm. luminescence (arb. units)
1,4
1,2
1,0
0,8
0,6
0,4
0,2
0,0
Single crystal
Thin film
V2+O
VCu
V2+O
VCu
1,8 2,0 2,2 2,4 2,6 2,8 3,0
Energy (eV)

Materials for Photonics

Formation of a self-trapped exciton and a non-bridging oxygen center in crystalline quartz grown from an NH4F solution under two-photon excitation.

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Georg Chikvaidze , University of Latvia Institute of Solid State Physics
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When irradiated with a focused ArF excimer laser beam (193 nm) at 15 K, a self-trapped exciton and a non-bridging oxygen center are formed in a quartz crystal grown from an NH4F solution. In quartz, grown from an alkaline solution, only self-trapped excitons are formed [1.2]. The STE spectrum consists of two strongly overlapping subbands at 2.7 and 2.5 eV with different polarization orientations and slightly different thermal quenching activation energies, however the non-bridging oxygen provides the red luminescence band (Fig.1). Such a center is primarily characteristic of the glassy state of SiO2, well known as a non-bridging oxygen hole center (NBOHC, oxygen dangling bond) [3], while NBOHC has also been observed in heavily irradiated (neutron, fast electron) quartz crystals (not grown from NH4F) (e.g., [4]). Currently, it is formed as stable at room temperature in a pure electron-hole two-photon excitation process at ~15 K in quartz grown from NH4F. If excitation is carried out by a focused ArF laser beam at a temperature of about 80 K, the resulting centers are unstable at higher temperatures. When measured at low temperature (15 K), the luminescence spectrum revealed a broad band in the 640–750 nm region, superimposed by at least five narrow lines: three strong ones at 648.5, 650.0, and 666.5 nm, and two weak lines at 655.5 and 674.7 nm. The studied crystal contains OH groups, and the IR spectrum consists of a series of intense narrow lines in the 3680–3600 cm^{-1} region. The formation of NBOHC-like centers under the action of ArF laser photons in our unirradiated samples is apparently due to the photolysis of hydroxyl groups in a two-photon process with product stabilization due to the low temperature.

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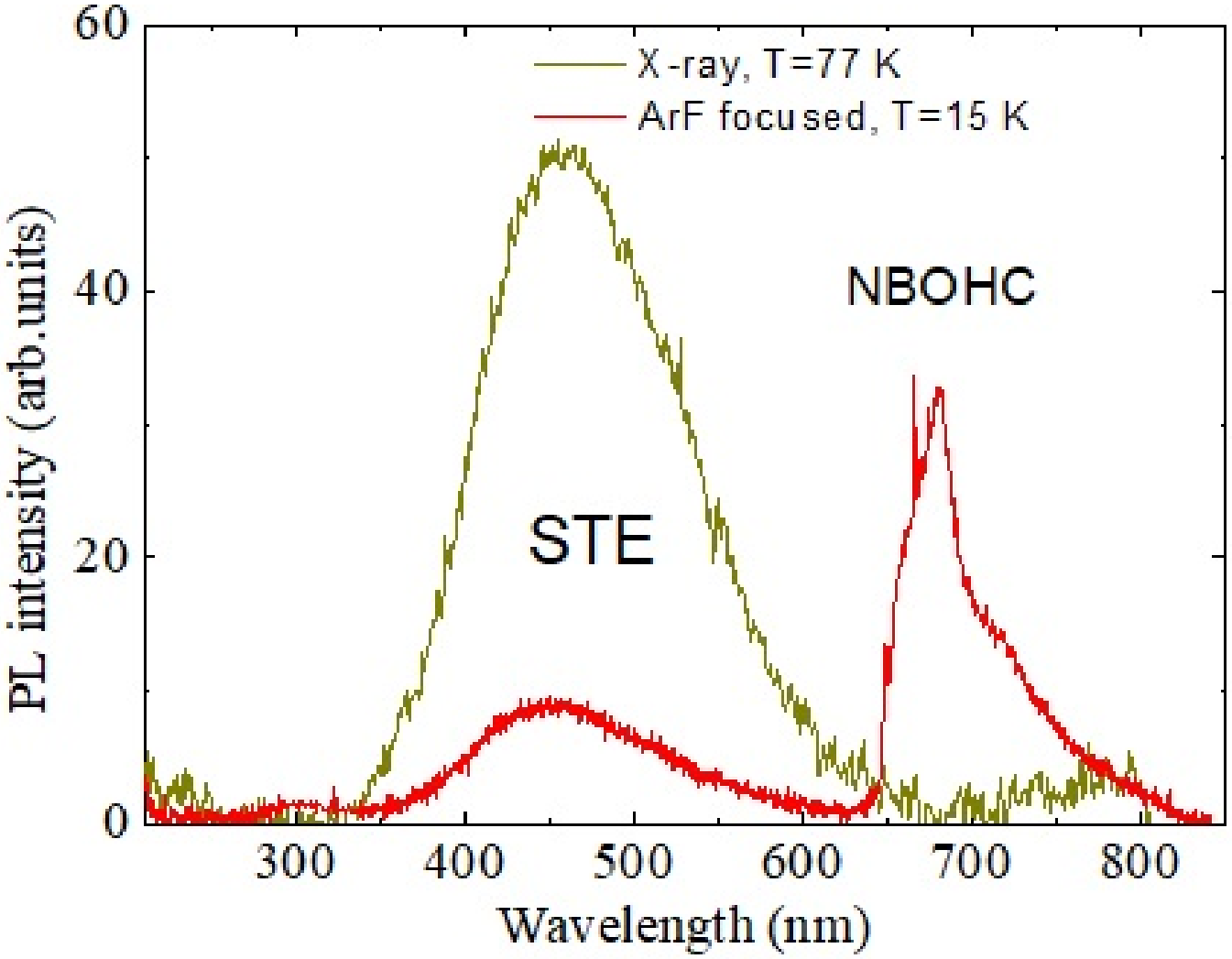
Keywords

excimer laser, quartz crystal, self-trapped exciton, non-bridging oxygen hole center


X-ray, T=77 K
ArF focused, T=15 K
NBOHC
STE
PL intensity (arb.units)
Wavelength (nm)
0
20
40
60
300
400
500
600
700
800

Materials for Energy

Transparent WO_3/TiO_2 Nanocomposite Coatings with Enhanced Photochromic Switching for Smart Window Applications

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Aleksandrs Novikovs , Institute of Solid state Physics University of Latvia
Ligita Ostrovska , Institute of Solid State Physics, University of Latvia
Anastasija Nikolajeva , Institute of Solid State Physics, University of Latvia
Sergejs Fomins , Institute of Solid state Physics University of Latvia
Boris Polyakov , Institute of Solid state Physics University of Latvia

The rapid growth of global civilisation and industry has intensified the energy crisis, stimulating research in nanomaterials and nanotechnology for sustainable solutions [1]. Photochromic organic materials, which change colour and self-bleach under varying light conditions, are promising for smart window applications [2]. However, their use is limited by slow switching and poor long-term stability. Therefore, attention is shifting to inorganic materials, which offer better thermal and chemical stability, non-toxicity, and lower cost. Tungsten oxide (WO_3) is one of the most studied candidates [3], but its films still show limited optical modulation, slow response, and long bleaching times. Current strategies aim to improve performance by enhancing light absorption and charge-carrier mobility through microstructure control, nanoparticle size and morphology optimisation, doping, and improved polymer matrices for greater stability and transparency.

In this work, an optimized approach for synthesizing photochromic WO_3 nanoparticles and fabricating composite coatings with improved optical properties was developed. WO_3 nanoparticles were synthesized using the polyol method due to its simplicity, low cost, and reproducibility. The formation of a TiO_2-like shell on WO_3 particles enhanced the photochromic response, increasing optical modulation by about twofold due to improved charge transfer at the WO_3/TiO_2 interface. A two-component polymer matrix based on polyvinyl alcohol and triethylene glycol (PVA/TEG) was also developed. The addition of 11 wt.% TEG (relative to a 10% PVA solution) accelerated the bleaching process by approximately two times. The resulting WO_3/TiO_2 films in the PVA/TEG matrix show high transparency (up to 98%) and good stability: after 5 minutes of irradiation, the optical density increases by ~30%, while the initial transmittance recovers within 40–45 minutes.

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Keywords

Smart Window, photochromic coating, tungsten oxide,

Acknowledgements

PostDoc (1.1.1.9/LZP/1/24/020), SWITCH (1.1.1.3/1/24/A/049), Smart Windows for Zero Energy Buildings (SWEB) project

Materials for Photonics

Comparative study of nano-ceramic and single crystalline dosimetric phosphor YAlO3:Bi

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Oleksandr Poshyvak , Lviv Polytechnic National University, Lviv, Ukraine
Yulia Rumianseva , Łukasiewicz Research Network – Krakow Institute of Technology, Krakow, Poland
Marek Berkowski , Institute of Physics, Polish Academy of Science, Warsaw, Poland
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Interest in dosimetric phosphors with a high effective atomic number Z is due to the possibility of their joint use in tandem with widely used tissue-equivalent phosphors, which allows unknown radiation sources to be recognized by their different energy dependence of dosimetric sensitivity [1]. Yttrium-aluminium perovskite $YAlO_3$ (YAP), activated with Bi (YAP:Bi) with Z = 34.1, combines very well with BeO ceramics with Z = 7.2 in this approach [2]. Both exhibit optically stimulated luminescence (OSL) after irradiation, which is stimulated by blue light and emitted in the ultraviolet range.

This study is devoted to finding a method for producing the YAP:Bi phosphor in a solid state and concerns the sintering of ceramics from nano-powders synthesized by the sol-gel method and the growth of single crystals by the Czochralski method to meet the requirements for use in OSL dosimetry. Low-temperature synthesis allows for the introduction of larger amounts of Bi, which tends to evaporate. The concentration of Bi^{3+} in the detector was evaluated by the intensity of its photoluminescence at a wavelength of 325 nm when excited at 282 nm [3]. The subject of the comparative study was thermo-luminescence, OSL, and thermal fading. Despite the fact that the concentration of Bi^{3+} in the single crystal was significantly lower, the dosimetric sensitivity of the crystal and ceramics were comparable, but the crystal's accumulated dosimetric signal fading at storage in dark at room temperature was much lower – about 10%/3 months, as in the best commercially available dosimetric detectors.

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Keywords

dosimetry, phosphor, optically stimulated luminescence, YAP:Bi, thermal fading

Acknowledgements

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Ferroelectrics and Functional Materials

Synthesis, crystal structure and thermal behaviour of new high-entropy perovskite (Pr0.2Nd0.2Sm0.2Eu0.2Gd0.2)AlO3

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New high-entropy (HE) five-component aluminate perovskite with a nominal composition $(Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2}Gd_{0.2})AlO_3$ was synthesized as a single-phase material using a facile sol-gel citrate method. Phase pure perovskite material with an average crystallite size of 50 nm is formed after heat treatment of the product at 800 °C. With increasing annealing temperature, the crystallite size increases to 73 nm at 1200 °C and to 550 nm at 1500 °C. Full-profile Rietveld refinement proved the phase purity and the $GdFeO_3$-type perovskite structure with lattice parameters *a* = 5.3012 Å, *b* = 5.2917 Å and *c* = 7.4805 Å. Thermal expansion of HE $(Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2}Gd_{0.2})AlO_3$ perovskite between room temperature and 500 °C (Figure) exhibits pronounced anisotropic behaviour: the relative expansion along the *a*-axis is *ca* 1.5 times stronger than along the *b* and *c* axes. Within the studied temperature range, the unit cell dimensions of $(Pr_{0.2}Nd_{0.2}Sm_{0.2}Eu_{0.2}Gd_{0.2})AlO_3$ with an average ionic radius of 1.140 Å lie between the values of its constituent $REAlO_3$ compounds. This observation confirms that the lattice parameters and thermal expansion behaviour of the multi-component HE aluminate perovskites are in good agreement with the empirical relationships earlier established for the $REAlO_3$ series [1], indicating that the crystal structure parameters of HE perovskite materials are mainly governed by the geometrical factor.

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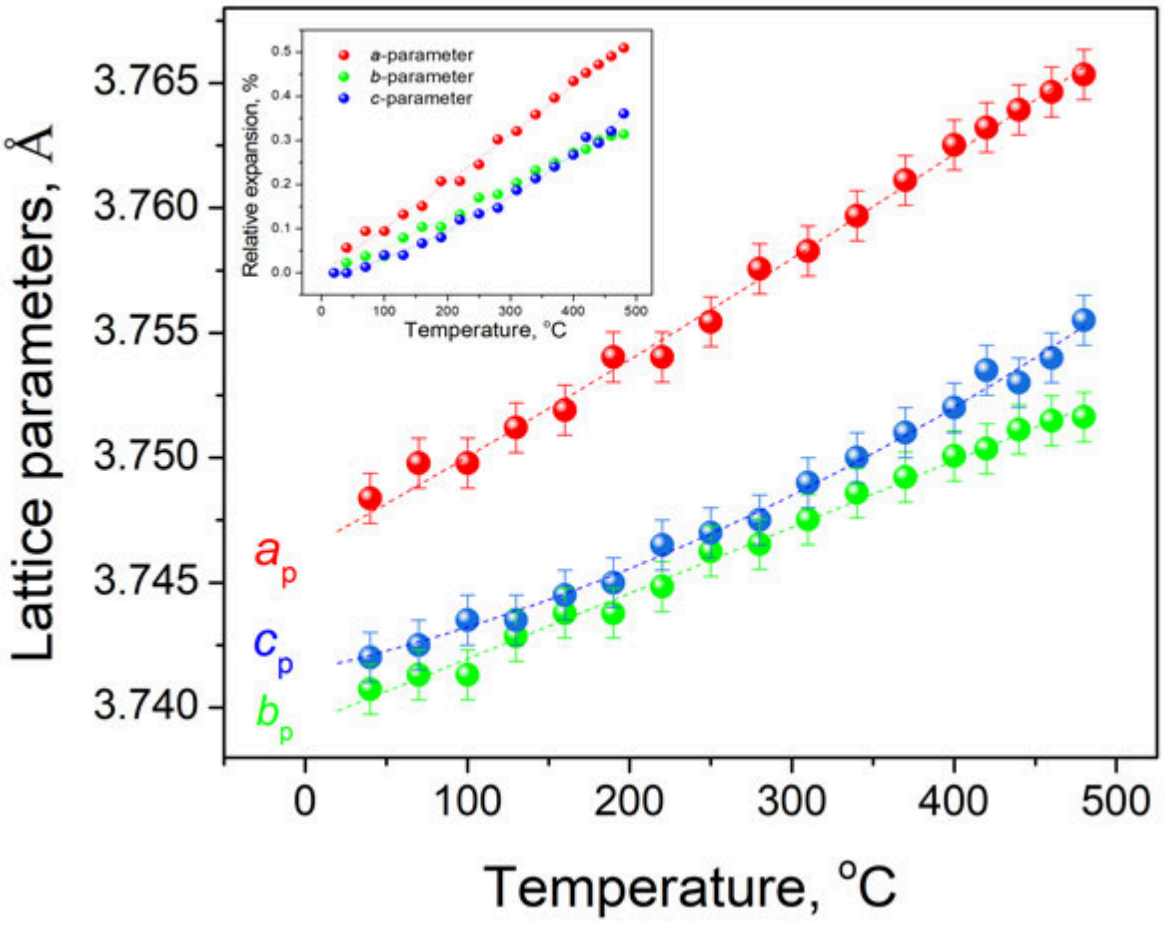
Keywords

High-entropy perovskites, aluminates, crystal structure, thermal expansion

Acknowledgements

The work was funded by the National Research Foundation of Ukraine under grant no. 2025.07/0218 “Engineering of structure, thermal behaviour and electronic properties of new high-entropy functional materials based on rare earth oxides using the concept of configurational entropy”.



Materials for Photonics

Comparative Study of Optical Absorption Uniformity in YAG:Cr^{4+} Epitaxial Film and Single Crystal

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Ihor Syvorotka , 1) Lviv Polytechnic National University, Lviv, Ukraine; 2) Scientific Research Company "Electron-Carat", Lviv, Ukraine;
Ivan Kolodiy , Lviv Polytechnic National University, Lviv, Ukraine

Chromium-doped yttrium aluminum garnet (YAG:Cr^{4+}) is a promising functional material due to its near-infrared absorption and potential application in laser-related devices [1]. In this work, a comparative study of the spatial distribution of optical absorption in a YAG:Cr^{4+} epitaxial film grown by liquid phase epitaxy (LPE) and a bulk YAG:Cr^{4+} single crystal was performed. The measurements were carried out by scanning the sample surface with recording the local optical absorption coefficient at a wavelength of 1064 nm, corresponding to Cr^{4+}-related absorption.

The results reveal a pronounced difference in the lateral homogeneity of the two materials. The epitaxial film demonstrates nearly constant absorption over the scanned area, indicating a high degree of spatial uniformity. In contrast, the bulk single crystal exhibits a significant variation of the absorption coefficient across the sample surface, evidencing noticeable optical inhomogeneity. In addition to the improved uniformity, the absolute value of the absorption coefficient in the epitaxial film is several times higher than that measured in the crystal.

These findings show that the epitaxial YAG:Cr^{4+} film possesses clear advantages over the bulk crystal in terms of both homogeneity and Cr^{4+}-related absorption strength. The observed behavior indicates the strong potential of epitaxial YAG:Cr^{4+} structures for photonic and laser applications, where spatially uniform optical properties are essential for stable and reproducible device performance.

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Keywords

YAG:Cr^{4+}, epitaxial film, single crystal, optical absorption, spatial uniformity

Acknowledgements

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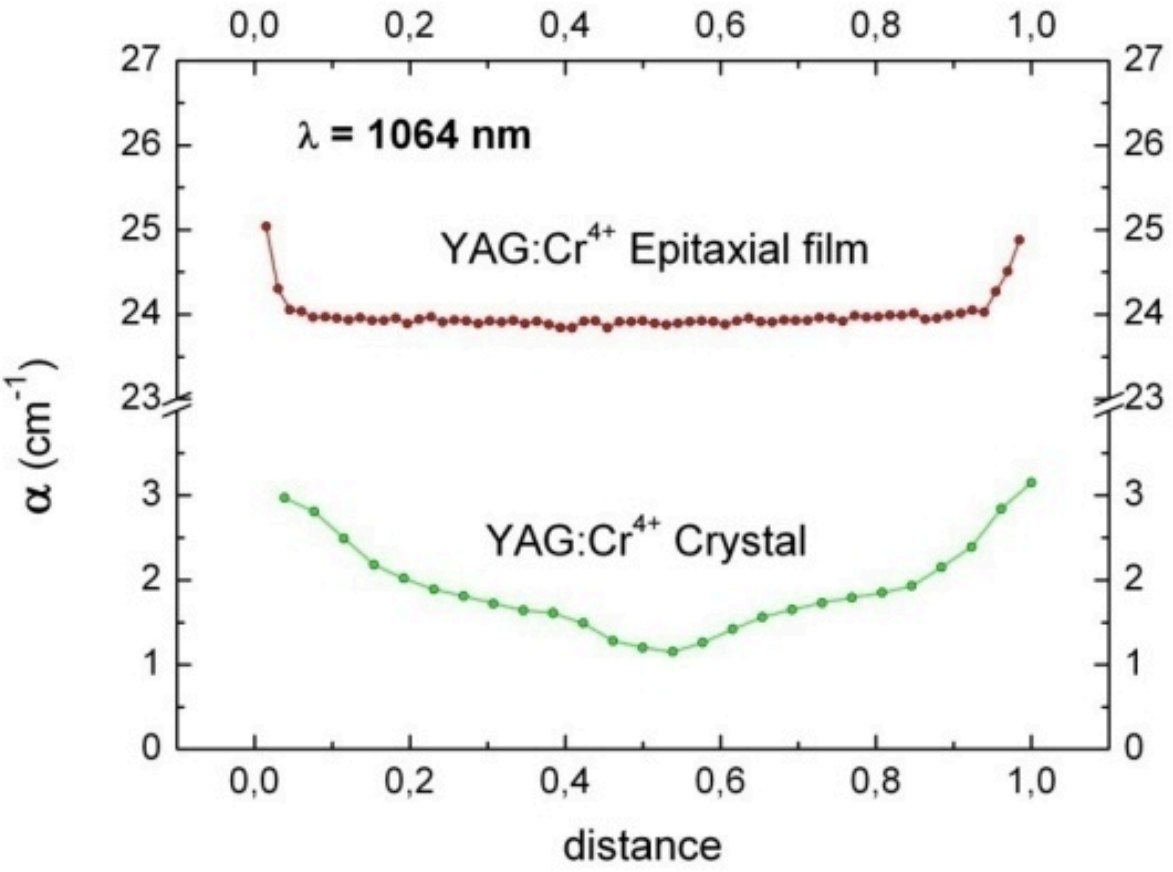
λ = 1064 nm
YAG:Cr4+ Epitaxial film
YAG:Cr4+ Crystal
α (cm-1)
distance
0,0
0,2
0,4
0,6
0,8
1,0
0
1
2
3
23
24
25
26
27

Materials for Energy

The influence of the high energy (12,5 MeV) electron irradiation on optical materials with Mg-spinel structure

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Nataliya Svatiuk , Institute of Electron Physics, National Academy of Sciences of Ukraine, Uzhhorod, Ukraine
Vasyl Hreb , Lviv Polytechnic National University, Lviv, Ukraine
Yulia Rumiantseva , Łukasiewicz Research Network – Krakow Institute of Technology, Krakow, Poland
Yaroslav Zhydachevskyy , Institute of Physics, Polish Academy of Science, Warsaw, Poland
Volodymyr Maslyuk , Institute of Electron Physics, National Academy of Sciences of Ukraine, Uzhhorod, Ukraine

Transparent Mg-spinel ceramics is one of the key optical materials for diagnostic windows in fusion technology and must be able to withstand intense particle irradiation, including neutron fluxes. Radiation resistance is also crucial for the use of transparent spinel ceramics in optical windows for spacecraft.

This study is devoted to investigation of the optical properties of ceramics sintered by HPHT method from $MgAl_2O_4$ spinel powder produced by high temperature solid phase synthesis and the changes induced with electron irradiation which simulates the high energy particle bombardment.

The irradiation was performed with electrons of 12.5 MeV energy using microtron M30 accelerator up to fluence 10^{17} cm^{-2} with the flux in range 10^{12} – 10^{13} $cm^{-2}{\cdot}s^{-1}$. The temperature of the samples during irradiation did not exceed 60 °C, which was achieved by blowing nitrogen over them during evaporation. The obtained results are compared with results of similar investigation published earlier.

Keywords

Spinel, transparent ceramics, electron irradiation, accelerator,

Acknowledgements

The study has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (GA No 101052200 EUROfusion) and was partially co funded by the Polish Ministry of Science and Higher Education (project No 602430) and the Ukrainian-Latvian Joint Programme of Scientific and Technological Cooperation (project 0125U003462 and LV-UA/2025/12).

Theoretical Modeling of Functional Materials and Devices

ML-Guided Screening of Heterojunction Photocatalysts for Green Hydrogen Production

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Serik Nurkenov , Department of Physical and Mathematical Sciences and Informatics, Astana International University, Astana, 010017, Kazakhstan
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Anatoli Popov , Institute of Solid State Physics, University of Latvia, Riga, LV-1063, Latvia

Photocatalytic hydrogen production from water splitting is a promising route for sustainable solar-to-fuel conversion, yet the rational design of efficient photocatalysts, especially heterojunction systems that enhance visible-light absorption and charge separation, remains challenging due to the vast combinatorial design space. Here we present a robust, broadly applicable multistep workflow that integrates density functional theory (DFT) with machine learning (ML) to accelerate the discovery of high-performance heterojunction photocatalysts for green hydrogen generation. We construct a large candidate library via data preprocessing and materials enumeration, followed by targeted DFT calculations on a representative subset to obtain key descriptors related to water-splitting performance, including band-edge alignment relative to redox potentials, charge-transfer driving force at the interface, adsorption energetics of relevant surface intermediates, and stability indicators. The resulting dataset is used to train and benchmark multiple ML regressors, including random forest, support vector regression, kernel ridge regression, and neural-network models. Model accuracy and generalization are improved through feature engineering across atomistic, structural, and electronic factors, recursive feature elimination, hyperparameter optimization, and leave-one-out validation. The best-performing model is then applied to predict properties for the remaining candidates, enabling high-throughput screening and prioritization for subsequent DFT refinement and experimental validation. Finally, we analyze feature importance to identify the dominant structure-property relationships governing hydrogen evolution activity in heterojunction photocatalysts.

Keywords

photocatalysis, hydrogen, machine learning

Acknowledgements

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Technologies and Devices

Crystal structure and mechanical properties of ALD-grown and thermally treated hafnium oxide–silicon oxide composite films

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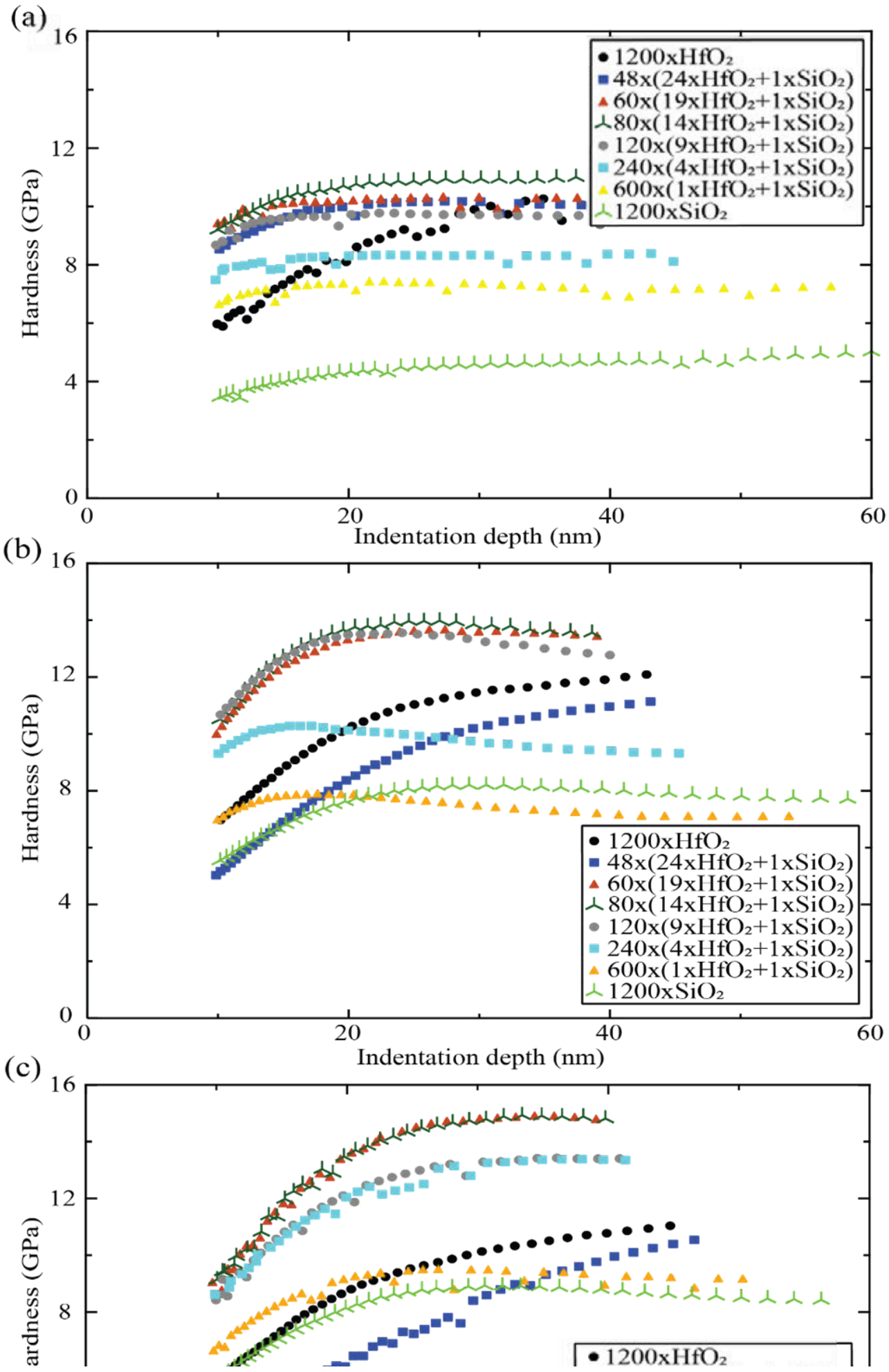
To the best of our knowledge, this study presents the first investigation into the mechanical properties of annealed SiO_2-doped HfO_2 thin films grown on Si substrates by atomic layer deposition, with doping levels ranging from 5 to 54.5 mol%. Tetrakis(ethylmethylamido)hafnium(IV) (TEMAHf) and hexakis(ethylamino)disilane (HEADS) were employed as precursors, with oxygen plasma serving as the oxidant. Furthermore, we report the unprecedented observation of a minor orthorhombic phase in 150 nm-thick films, a finding not previously documented in the literature.

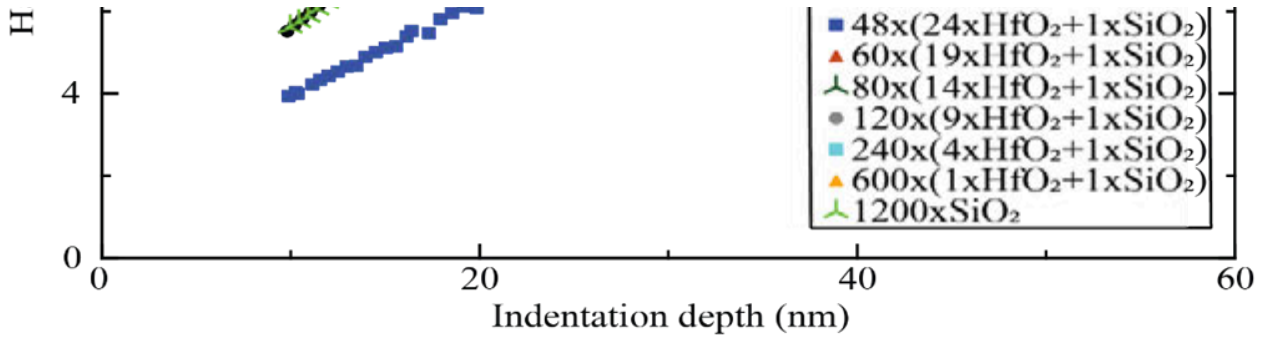
This work systematically examines the interplay between crystal structure, chemical composition, and mechanical properties in the deposited films. As illustrated in Figure 1, higher annealing temperatures correlate with highest enhanced hardness values found. On average, heat treatment increased film hardness by 15%, although the elastic modulus remained largely unaffected. Our results reveal that HfO_2 films exhibiting a mixture of cubic and tetragonal phases possess superior mechanical properties, with a maximum hardness value of 14.1 GPa.

These findings hold considerable relevance for researchers and engineers in the fields of nano- and micro-electromechanical systems (NEMS/MEMS), as well as for those involved in the development of ALD thin films for protective coatings.

Keywords

atomic layer deposition, nanoindentation, heat treatment


(a)
Hardness (GPa)
Indentation depth (nm)
1200xHfO2
48x(24xHfO2+1xSiO2)
60x(19xHfO2+1xSiO2)
80x(14xHfO2+1xSiO2)
120x(9xHfO2+1xSiO2)
240x(4xHfO2+1xSiO2)
600x(1xHfO2+1xSiO2)
1200xSiO2
(b)
Hardness (GPa)
Indentation depth (nm)
1200xHfO2
48x(24xHfO2+1xSiO2)
60x(19xHfO2+1xSiO2)
80x(14xHfO2+1xSiO2)
120x(9xHfO2+1xSiO2)
240x(4xHfO2+1xSiO2)
600x(1xHfO2+1xSiO2)
1200xSiO2
(c)
ardness (GPa)
1200xHfO2



Ferroelectrics and Functional Materials

Photothermally Activated Shape-Memory Polymer–Silver Nanoparticle Composites for Light-Triggered 3D-Printed Actuators

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Photothermally responsive shape-memory polymers enable remote and localized actuation by converting light into heat through embedded photothermal fillers. In this work, a plant-derived acrylate shape-memory polymer composite containing silver nanoparticles was developed and fabricated into functional structures using vat photopolymerization. The Ag nanoparticles were synthesized via a microwave-assisted solvothermal method and incorporated into a bio-based acrylate resin derived from acrylated rapeseed oil.

The influence of nanoparticle incorporation on curing behaviour, thermomechanical properties, optical absorption, and photothermal heating was investigated using FTIR spectroscopy, photorheology, dynamic mechanical analysis, tensile testing, and infrared thermography. The presence of AgNPs reduced the effective curing rate and final conversion due to optical attenuation during photopolymerization. As a result, the composite exhibited reduced stiffness and tensile strength compared to the neat polymer, while maintaining high deformability required for shape-memory functionality.

As a proof of concept, 3D-printed ring structures showed repeatable light-induced shape recovery. These results demonstrate that AgNP-loaded plant-based polymers provide a sustainable platform for remotely actuated shape-memory devices, with potential applications in soft robotics, deployable structures, and minimally invasive biomedical systems.

Keywords

shape-memory polymer, photothermal, silver nanoparticles, 3D printing, plant-based polymers

Acknowledgements

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Ferroelectrics and Functional Materials, Technologies and Devices

Atomic Layer Deposition of ZnO Nanostructures onto Glass Wool

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The ZnO is known as a cheap, non-toxic, chemically stable, photosensitive and thermoelectric material. The physical properties of ZnO can be enhanced by increasing the surface-to-volume ratio by nanostructuring [1]. The atomic layer deposition (ALD) method was widely used for deposition of ZnO nanostructures onto materials with different morphologies [2, 3].

Since ZnO nanostructures, synthesized by the ALD technique, follow the substrate morphology, it is expected that ALD ZnO deposition can replicate the fibrous morphology of substrates such as glass wool. Due to its low thermal conductivity, glass wool is widely used as an effective thermal insulation material to increase the energy efficiency of buildings by reducing heat loss. Additionally, it is thermally stable up to 600 °C, chemically inert, flexible, and the fibrous structure provides a large surface area, making it a good substrate for the synthesis of nanostructures. In this study presented ZnO/glass wool structures may find applications in thermoelectric thermal insulation panels, gas filters, gas sensors, etc.

ZnO nanostructured layers of different thicknesses were synthesized on glass wool substrates by using the atomic layer deposition method. Morphology and structure of the nanostructures were characterized using scanning electron microscopy, energy X-ray dispersive spectroscopy, X-ray diffractometry. Electrical conductivity and thermoelectric properties of nanostructures were inspected depending on the deposited ZnO layer thickness.

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Keywords

zinc oxide, atomic layer deposition, glass wool

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Theoretical Modeling of Functional Materials and Devices

EXAFS spectroscopy study of the temperature-dependent lattice dynamics of wurtzite ZnO

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Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy is an experimental technique used to investigate the local atomic structure and lattice dynamics of materials. In this study, it was applied to examine the temperature-dependent local lattice dynamics of polycrystalline wurtzite-type ZnO [1].

The experiments [2] were performed in transmission mode at the Zn K-edge in the temperature range 300–1200 K at the BALDER beamline of the MAX IV Laboratory [3]. For completeness, low-temperature (10–300 K) EXAFS data from a previous study [4] were also included. Two approaches were used to analyze the experimental data: (i) conventional multi-component fitting within the single-scattering approximation [5] and (ii) the reverse Monte Carlo (RMC) method combined with an evolutionary algorithm [6].

Analysis of the EXAFS contributions from the first two coordination shells (Zn–O and Zn–Zn) using the first approach allowed determination of the temperature dependence of the mean-square relative displacements (MSRDs). Effective force constants describing the stiffness of local chemical bonds were derived for each shell using the Einstein model [5]. Possible anharmonicity of the interatomic potential and distortion of the first coordination shell were evaluated from the third cumulant. The RMC method extended the analysis to ~7 Å, including contributions from about 15 coordination shells, and enabled determination of the effective force constant as a function of interatomic distance.

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Keywords

ZnO, wurtzite, X-ray absorption spectroscopy, reverse Monte Carlo simulations, lattice dynamics

Acknowledgements

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Ferroelectrics and Functional Materials

Phase-Selective Synthesis of EuS2 and Eu3S4 via the Boron Chalcogen Mixture Method

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In the present work, the phase-selective synthesis of EuS_2 and Eu_3S_4 was achieved *via* the phase conversion from $Eu(OH)_3$ nanorods by the Boron Chalcogen Mixture (BCM) Method. For the synthesis, two separate quartz tubes containing the $Eu(OH)_3$ precursor and the S-B mixture, respectively, were placed in a larger-diameter quartz tube, evacuated, and sealed. For the heat-treatment procedure, the obtained ampules were placed vertically in the muffle furnace and annealed at an appropriate temperature for 48 h.

The resulting powders were characterized by powder X-ray diffraction analysis (XRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and magnetic susceptibility measurements. *In-situ* temperature-dependent XRD measurements between RT and 500 °C revealed no detectable changes in the phase composition or crystal structure of the materials. Almost linear increase of the lattice parameters and unit cell volume was observed. EuS_2 showed clear anisotropic thermal expansion in different crystallographic directions: relative expansion along *c*-axis is considerably higher as along *b*- and *a*-axes.

Keywords

EuS2; Eu3S4; Boron Chalcogen Mixture Method

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Materials for Energy, Theoretical Modeling of Functional Materials and Devices

Probing the Local Structure and Lattice Dynamics of Rhenium-Substituted VO_2 with Universal Machine Learning Potentials

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Doping vanadium dioxide (VO_2) with rhenium provides an effective way to tune the temperature of its insulator–to–metal transition [1], making this material attractive for applications such as thermochromic smart windows. However, the incorporation of rhenium into the VO_2 lattice and its impact on the local structure and lattice dynamics remain insufficiently understood. In particular, the coordination environment of rhenium and its influence on the host matrix require further clarification.

Universal machine learning interatomic potentials (uMLIPs) have recently emerged as powerful and computationally efficient tools for studying the structure and dynamics of materials beyond the limits of direct first-principles simulations. However, their out-of-the-box performance for strongly correlated transition-metal oxides such as VO_2 has not been systematically evaluated.

In this work, we investigate rhenium-substituted VO_2 ($Re_xV_{1-x}O_2$) using uMLIPs [2] and benchmark the results against first-principles calculations. We assess how well these potentials reproduce both the structure of VO_2 and the local environment of substituted rhenium atoms. Furthermore, we examine how limited fine-tuning of the uMLIPs using small datasets of first-principles calculations improves their accuracy. The capabilities and current limitations of uMLIPs for describing structural properties and lattice dynamics in this class of materials are discussed.

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Keywords

RexV1–xO2 solid solution, structure, universal machine learning interatomic potentials, fine-tuning

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Microfluidics and Biomedical technologies

Engineering Scalable Aptamer-Gold Interfaces for Rapid Malaria Diagnostics

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Malaria remains a global health challenge, further exacerbated by climate change and increased human mobility, which contribute to the re-emergence of the disease in non-endemic regions [1-3]. Currently deployed rapid diagnostic tests (RDTs) rely on antibodies as recognition elements. However, antibodies are prone to thermal degradation and exhibit high batch-to-batch variability, limiting their robustness in field conditions. Within the BioPhoT framework, this work presents a transition towards a more robust diagnostic platform using DNA aptamers as synthetic, thermally stable molecular recognition elements [4].

This study focuses on the industrial scalability of self-assembled monolayers (SAMs) on gold-functionalized sensor substrates. The sensing interface is based on thiol-modified DNA aptamers that self-assemble on gold to form highly oriented and densely packed probe layers, enabling selective pathogen capture [5].

To facilitate practical deployment, the biosensor is implemented as a cartridge-based diagnostic device. The disposable cartridge integrates the sensing surface containing the aptamer-based recognition stack, while signal acquisition is performed using an external optical reader based on spectrophotometric detection. This configuration enables rapid and quantitative signal readout while maintaining a simple and user-friendly operational workflow.

We present the architectural design of this modular biosensing prototype, emphasising a plug-and-play cartridge format compatible with portable instrumentation and high-throughput laboratory workflows. By replacing biological recognition elements with chemically synthesised aptamers, this platform offers a more stable and cost-effective approach for next-generation diagnostic devices, improving reliability under challenging environmental conditions.

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Keywords

Aptamer biosensor, point-of-care malaria detection, self-assembled monolayers, thiol–gold chemistry

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PHOTO-ASSISTED ENERGY STORAGE IN AQUEOUS ZINC-ION BATTERIES USING BI2SE3–MWCNT CATHODES

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The growing demand for safe and reliable energy storage technologies highlights the need for alternatives to currently dominant lithium-ion batteries that are safer, environmentally sustainable, and cost-effective. Aqueous zinc batteries present a promising solution. Zinc is abundant and fully recyclable, while water-based electrolytes improve operational safety and reduce health risks. These characteristics make aqueous zinc-ion batteries an attractive approach for sustainable energy storage. In addition to conventional charging using external power sources, photo-assisted charging enables partial battery charging using sunlight, reducing dependence on external energy input. Integrating a photocathode into an electrochemical storage system could also eliminate the need for separate photovoltaics and storage units by combining them within a single device. Semiconductor materials such as Bi_2Se_3 are promising electrode candidates due to their layered structure, which facilitates efficient ion intercalation. Previous studies have shown that Bi_2Se_3 carbon nanotube heterostructures exhibit excellent electrochemical performance in lithium-ion batteries [1]. In this work, Bi_2Se_3 – MWCNT heterostructures were investigated as photocathodes for aqueous zinc-ion batteries. The heterostructures were fabricated by physical vapor deposition of Bi_2Se_3 nanostructures onto a spray-coated MWCNT network on indium tin oxide glass. Morphology and composition were analyzed using scanning electron microscopy and energy-dispersive X-ray spectroscopy, while electrochemical performance was evaluated by cyclic voltammetry and galvanostatic charge–discharge measurements under dark and illuminated conditions. The results showed increased battery capacity under illumination, demonstrating the potential of Bi_2Se_3 – MWCNT heterostructures for photo-assisted zinc-ion batteries.

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Keywords

Bi2Se3, Zinc batteries, photo-assisted, aqueous electrolyte.

Acknowledgements

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Theoretical Modeling of Functional Materials and Devices

Bismuth modified SrTiO3 perovskites for green hydrogen production: DFT studies

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$SrTiO_3$ and $Bi_4Ti_3O_{12}$ are promising materials for sustainable hydrogen production via photocatalysis due to their excellent catalytic properties and structural versatility. The layered $Bi_4Ti_3O_{12}$ structure promotes the growth in two-dimensional (2D) morphology, while the symmetrical crystal structure of $SrTiO_3$ does not facilitate the spontaneous formation of 2D nanostructures. However, due to their structural similarity, combined with favorable dissolution and transformation chemistries under hydrothermal conditions, $Bi_4Ti_3O_{12}$ template nanoplatelets can gradually transform into $SrTiO_3$ nanoplatelets leading to materials with enhanced photocatalytic performance [1,2].

This study investigates the electronic and geometric properties of such materials using hybrid DFT calculations as implemented in Crystal23. We have demonstrated the band gap decrease with Bi incorporation into $SrTiO_3$ resulting in either $SrTiO_3/Bi_4Ti_3O_{12}$ heterostructure or BiO monolayer in $SrTiO_3$ models. The theoretical studies are supported by the atomic scale characterization of the $SrTiO_3/Bi_4Ti_3O_{12}$ and $SrTiO_3$ nanoplatelets.

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Keywords

SrTiO3, heterostructure, DFT calculations

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